Gaussian decay for a difference of traces of the Schrödinger semigroup associated to the isotropic harmonic oscillator.

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Abstract

This paper deals with the derivation of a sharp estimate on the difference of traces of the one-parameter Schrödinger semigroup associated to the quantum isotropic harmonic oscillator. Denoting by $H_{\infty,\kappa}$ the self-adjoint realization in $L^2(\mathbb{R}^d)$, $d \in \{1,2,3\}$ of the Schrödinger operator $-\frac{1}{2}\Delta + \frac{1}{2}\kappa^2|\mathbf{x}|^2$, $\kappa > 0$ and by $H_{L,\kappa}$, $L > 0$ the Dirichlet realization in $L^2(\Lambda_L^d)$ where $\Lambda_L^d := \{\mathbf{x} \in \mathbb{R}^d : -L/2 < x_l < L/2, l = 1,\dots,d\}$, we prove that the difference of traces $\mathrm{Tr}_{L^2(\mathbb{R}^d)}\mathrm{e}^{-tH_{\infty,\kappa}} - \mathrm{Tr}_{L^2(\Lambda_L^d)}\mathrm{e}^{-tH_{L,\kappa}}$, $t > 0$ has a Gaussian decay in L for L sufficiently large. The estimate we derive is sharp in the sense that its behavior when $\kappa \downarrow 0$ and $t \downarrow 0$ is similar to the one given by $\mathrm{Tr}_{L^2(\mathbb{R}^d)}\mathrm{e}^{-tH_{\infty,\kappa}} = (2\sinh(\frac{\kappa}{2}t))^{-d}$. Further, we give a simple application within the framework of quantum statistical mechanics.

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Contents

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1 Introduction.

1.1 The setting and the main result.

For any $d \in \{1,2,3\}$ and $L \in (0,\infty)$, denote $\Lambda_L^d := \{\mathbf{x} \in \mathbb{R}^d : -\frac{L}{2} < x_l < \frac{L}{2},\ l = 1,\dots,d\}$ and $|\Lambda_L^d|$ its Lebesgue-measure. On $\mathcal{C}_0^\infty(\Lambda_L^d)$, define $\forall \kappa > 0$ the family of operators:

$$H_{L,\kappa} := \frac{1}{2}\left(-i\nabla_{\mathbf{x}}\right)^2 + \frac{1}{2}\kappa^2|\mathbf{x}|^2. \tag{1.1}$$

It is well-know that $\forall \kappa > 0$, (1.1) extends to a family of self-adjoint and bounded from below operators $\forall L \in (0,\infty)$, denoted again by $H_{L,\kappa}$, with domain $D(H_{L,\kappa}) = W_0^{1,2}(\Lambda_L^d) \cap W^{2,2}(\Lambda_L^d)$. Obviously this definition corresponds to choose Dirichlet boundary conditions on the boundary $\partial\Lambda_L^d$. Since the inclusion $W_0^{1,2}(\Lambda_L^d) \hookrightarrow L^2(\Lambda_L^d)$ is compact, then $\forall \kappa > 0$ $H_{L,\kappa}$ has a purely discrete spectrum with an accumulation point at infinity.

When Λ_L^d fills the whole space (when $L \uparrow \infty$), define $\forall \kappa > 0$ on $\mathcal{C}_0^\infty(\mathbb{R}^d)$ the family of operators:

$$H_{\infty,\kappa} := \frac{1}{2}\left(-i\nabla_{\mathbf{x}}\right)^2 + \frac{1}{2}\kappa^2|\mathbf{x}|^2. \tag{1.2}$$

From [14, Thm. X.28], $\forall \kappa > 0$ (1.2) is essentially self-adjoint and its self-adjoint extension, denoted again by $H_{\infty,\kappa}$, is semi-bounded. By [15, Thm. XIII.16], the spectrum of $H_{\infty,\kappa}$ is purely discrete with eigenvalues increasing to infinity. From the one-dimensional problem, the eigenvalues and eigenfunctions of the multidimensional case can be written down explicitly. The eigenvalues of the one-dimensional problem are all non-degenerate and given by, see e.g. [4, Sec. 1.8]:

$$\epsilon_{\infty,\kappa}^{(s)} := \kappa\left(s + \frac{1}{2}\right), \quad s \in \mathbb{N}. \tag{1.3}$$

The corresponding eigenfunctions, which form an orthonormal basis in $L^2(\mathbb{R})$ read as:

$$\forall x \in \mathbb{R}, \quad \phi_{\infty,\kappa}^{(s)}(x) := \frac{1}{\sqrt{2^s s!}}\left(\frac{\kappa}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{\kappa}{2}x^2}\mathcal{H}_s\left(\sqrt{\kappa}x\right), \quad s \in \mathbb{N}, \tag{1.4}$$

where $\mathcal{H}_s$, $s \in \mathbb{N}$ are the Hermite polynomials defined by: $\mathcal{H}_s(x) := (-1)^s \mathrm{e}^{x^2}\frac{\mathrm{d}^s}{\mathrm{d}x^s}(\mathrm{e}^{-x^2})$, $\forall x \in \mathbb{R}$. The eigenvalues and eigenfunctions of the multidimensional case (i.e. $d = 2,3$) are respectively related to those of the one-dimensional case by:

$$E_{\infty,\kappa}^{(\mathbf{s})} := \sum_{j=1}^d \epsilon_{\infty,\kappa}^{(s_j)} = \kappa\sum_{j=1}^d\left(s_j + \frac{1}{2}\right), \quad \mathbf{s} = \{s_j\}_{j=1}^d \in \mathbb{N}^d, \tag{1.5}$$

$$\psi_{\infty,\kappa}^{(\mathbf{s})}(\mathbf{x}) := \prod_{j=1}^d \phi_{\infty,\kappa}^{(s_j)}(x_j), \quad \mathbf{x} = \{x_j\}_{j=1}^d \in \mathbb{R}^d. \tag{1.6}$$

From (1.3)-(1.5) and by the use of the min-max principle, one has for any $L \in (0,\infty)$:

$$\forall \kappa > 0, \quad \inf\sigma\left(H_{L,\kappa}\right) \geq \inf\sigma\left(H_{\infty,\kappa}\right) = E_{\infty,\kappa}^{(\mathbf{0})} = d\epsilon_{\infty,\kappa}^{(0)} > 0, \quad \epsilon_{\infty,\kappa}^{(0)} := \frac{\kappa}{2}.$$

Let us turn to the one-parameter strongly-continuous semigroup (the so-called C_0-semigroup in the Hille-Phillips terminology [11]) generated by the operators introduced above. At finite-volume, it is defined $\forall L \in (0,\infty)$ and $\forall \kappa > 0$ by $\{G_{L,\kappa}(t) := \mathrm{e}^{-tH_{L,\kappa}} : L^2(\Lambda_L^d) \to L^2(\Lambda_L^d)\}_{t\geq 0}$. It is a self-adjoint and positive operator on $L^2(\Lambda_L^d)$ by the spectral theorem and the functional calculus, see e.g. [18]. The same hold true for the one-parameter semigroup on the whole space $\{G_{\infty,\kappa}(t) := \mathrm{e}^{-tH_{\infty,\kappa}} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)\}_{t\geq 0}$. Moreover $\forall 0 < L \leq \infty$, $\forall \kappa > 0$ and $\forall t > 0$,

$G_{L,\kappa}(t)$ is a Gibbs semigroup, i.e. $G_{L,\kappa}(t)$ (resp. $G_{\infty,\kappa}(t)$) belongs to the Banach space of trace-class operators on $L^2(\Lambda_L^d)$ (resp. $L^2(\mathbb{R}^d)$), see [19, 2] and [20, Sec. 3]. A basic feature is the monotonicity property for the finite-volume trace, see Lemma A.4 in Sec. A:

$$\forall L \in (0,\infty), \quad \mathrm{Tr}_{L^2(\Lambda_L^d)}\left\{G_{L,\kappa}(t)\right\} \leq \mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(t)\right\} = \left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^{-d}, \quad \kappa > 0,\, t > 0.$$

Our main result is the following sharp estimate on the difference of traces of the semigroups:

Theorem 1.1. *$\forall d \in \{1,2,3\}$ there exists a constant $C_d > 0$ and a $\mathcal{L} \geq 1$ s.t. $\forall L \in [\mathcal{L},\infty)$, $\forall \kappa > 0$ and $\forall t > 0$:*

$$\begin{aligned}&\left|\mathrm{Tr}_{L^2(\Lambda_L^d)}\left\{G_{L,\kappa}(t)\right\} - \mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(t)\right\}\right| \\ &\qquad \leq C_d(1+t)^{2d+\frac{3}{2}}\left\{\left(1+\sqrt{\kappa}\right)^2 \mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(t)\right\} + \left(\frac{L}{\sqrt{t}}\right)^{d-1}\right\} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}. \end{aligned} \tag{1.7}$$

As a corollary of Theorem 1.1, one has the following estimate:

Corollary 1.2. *$\forall d \in \{1,2,3\}$ there exists a constant $C_d > 0$ and $\forall 0 < \kappa_0 < 1$ there exists a $\mathcal{L}_{\kappa_0} > 0$ s.t. $\forall L \in [\mathcal{L}_{\kappa_0},\infty)$, $\forall \kappa \in [\kappa_0,\infty)$ and $\forall t > 0$:*

$$\begin{aligned}&\left|\mathrm{Tr}_{L^2(\Lambda_L^d)}\left\{G_{L,\kappa}(t)\right\} - \mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(t)\right\}\right| \\ &\qquad \leq C_d\left(1+\sqrt{\kappa}\right)(1+\kappa)^d(1+t)^{3(d+\frac{1}{2})}\mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(t)\right\}\mathrm{e}^{-\frac{\kappa}{32}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}. \end{aligned} \tag{1.8}$$

Remark 1.3. The upper-bound in (1.7) is made up of two terms: the first one identifies with a bulk-like contribution, the second one with a boundary-like contribution.

Remark 1.4. The estimate in (1.7) is sharp in the sense that its behavior when $\kappa \downarrow 0$ and $t \downarrow 0$ is given by the term $\mathrm{Tr}_{L^2(\mathbb{R}^d)}\{G_{\infty,\kappa}(t)\} = (2\sinh(\frac{\kappa}{2}t))^{-d}$. We recall that $\sinh(x) \sim x$ when $x \downarrow 0$.

Remark 1.5. In the r.h.s. of (1.7), one can get rid of the polynomial growth in L (when $d > 1$) appearing in the second contribution via (A.16). This will give rise to an exponential growth of type $\exp(\frac{\kappa}{2}t)$, but the main singularity in $\kappa \downarrow 0$ and $t \downarrow 0$ is still given by the term $\mathrm{Tr}_{L^2(\mathbb{R}^d)}\{G_{\infty,\kappa}(t)\}$.

Remark 1.6. We stress the point that the upper bound in (1.8) cannot be derived directly from (1.7) due to the inequality $\sinh(\kappa t) \geq \kappa t$, $\forall \kappa, t > 0$. Moreover, the upper bound only has a polynomial growth in t. The price to pay to make appear the term $\mathrm{Tr}_{L^2(\mathbb{R}^d)}\{G_{\infty,\kappa}(t)\}$ as a common factor, is that for $0 < \kappa < 1$, the estimate holds for L large enough chosen accordingly (i.e. $L \geq cste/\sqrt{\kappa}$). Note that the $\mathcal{L}$ in Corollary 1.2 can be chosen uniformly in $\kappa \in [1,\infty)$.

Remark 1.7. In (1.7) and (1.8), the powers on the factors $(1+\sqrt{\kappa})$, $(1+\kappa)$, $(1+t)$ and the constant appearing in the argument of the exponential can be optimized.

1.2 An application in quantum statistical mechanics.

Consider a d-dimensional ideal quantum gas composed of a large number of non-relativistic spin-0 identical particles confined in the box Λ_L^d and trapped in an isotropic harmonic potential. Such a system is considered to figure out the Bose-Einstein condensation phenomenon created by cold alkali atom gases in magnetic-optical trap, see e.g. [13, Chap. 10] and references therein. Within the one-body approximation, the dynamics of a single Boson is determined by (1.1). Suppose that the system is at equilibrium with a thermal and particles bath. In the grand-canonical ensemble, let $(\beta, z, |\Lambda_L^d|)$ be the external parameters. Here, $\beta := (k_B T)^{-1} > 0$ is the 'inverse' temperature (k_B stands for the Boltzmann constant) and $z = \mathrm{e}^{\beta\mu}$ the fugacity (μ is the chemical potential). The finite-volume single-particle partition function is defined as, see e.g. [16]:

$$\Phi_{L,\kappa}(\beta) := \mathrm{Tr}_{L^2(\Lambda_L^d)}\left\{G_{L,\kappa}(\beta)\right\}, \quad \beta > 0. \tag{1.9}$$

The grand-canonical average number of particles at finite-volume is related to (1.9) by, see [3]:

$$\overline{N}_{L,\kappa}(\beta, z) := \sum_{l=1}^{\infty} z^l \Phi_{L,\kappa}(l\beta), \quad \beta > 0,\, z \in \left(0, \mathrm{e}^{\beta \inf \sigma(H_{L,\kappa})}\right). \tag{1.10}$$

Theorem 1.1 (resp. Corollary 1.2) allows to get the *large-volume behavior* of the single-particle partition function (resp. the grand-canonical average number of particles). Indeed, one gets $\forall 0 < \kappa_1 < \kappa_2 < \infty$, $\forall 0 < \beta_1 < \beta_2 < \infty$ and for any compact subset $K \subset (0, \mathrm{e}^{\beta_1 E_{\infty,\kappa_1}^{(\mathbf{0})}})$:

$$\Phi_{\infty,\kappa}(\beta) := \lim_{L\uparrow\infty} \Phi_{L,\kappa}(\beta) = \mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(\beta)\right\} = \frac{\mathrm{e}^{-\beta E_{\infty,\kappa}^{(\mathbf{0})}}}{\left(1-\mathrm{e}^{-\beta\kappa}\right)^d},$$

$$\overline{N}_{\infty,\kappa}(\beta, z) := \lim_{L\uparrow\infty} \overline{N}_{L,\kappa}(\beta, z) = \sum_{l=1}^{\infty} z^l \Phi_{\infty,\kappa}(l\beta),$$

uniformly in $(\kappa, \beta, z) \in [\kappa_1, \kappa_2] \times [\beta_1, \beta_2] \times K$. Moreover, one has the following asymptotics:

$$\Phi_{L,\kappa}(\beta) = \Phi_{\infty,\kappa}(\beta) + \mathcal{O}\left(\mathrm{e}^{-cL^2}\right),$$

$$\overline{N}_{L,\kappa}(\beta, z) = \overline{N}_{\infty,\kappa}(\beta, z) + \mathcal{O}\left(\mathrm{e}^{-cL^2}\right),$$

for some L-independent constant $c = c(\kappa, \beta) > 0$. We emphasize that the upper bound in (1.8) plays a crucial to prove the thermodynamic limit of (1.10) for any $z \in (0, \mathrm{e}^{\beta E_{\infty,\kappa}^{(\mathbf{0})}})$, see [3, Sec. A].

2 Proof of Theorem 1.1 and Corollary 1.2.

The starting-point consists in rewriting the difference between the traces involving the difference between the semigroup integral kernels. We refer the reader to Sec. A in which we have collected some basic properties on the semigroup kernel. Since $\forall L \in (0, \infty]$ and $\forall \kappa > 0$, $\{G_{L,\kappa}(t)\}_{t>0}$ is a Gibbs semigroup with a jointly continuous integral kernel $G_{L,\kappa}^{(d)}(\cdot\,,\cdot\,;t) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$, then:

$$\mathrm{Tr}_{L^2(\mathbb{R}^d)}\left\{G_{\infty,\kappa}(t)\right\} - \mathrm{Tr}_{L^2(\Lambda_L^d)}\left\{G_{L,\kappa}(t)\right\} = \mathscr{Y}_{L,\kappa}^{(d)}(t) + \mathscr{Z}_{L,\kappa}^{(d)}(t),$$

with $\forall d \in \{1, 2, 3\}$, $\forall L \in (0, \infty)$, $\forall \kappa > 0$ and $\forall t > 0$:

$$\mathscr{Y}_{L,\kappa}^{(d)}(t) := \int_{\Lambda_L^d} \mathrm{d}\mathbf{x}\, \left\{G_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{x}; t) - G_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{x}; t)\right\}, \tag{2.1}$$

$$\mathscr{Z}_{L,\kappa}^{(d)}(t) := \int_{\mathbb{R}^d \setminus \Lambda_L^d} \mathrm{d}\mathbf{x}\, G_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{x}; t). \tag{2.2}$$

Here, we used [8, Prop. 9]. Note that $\forall \kappa > 0$, $\forall t > 0$ the kernel $G_{\infty,\kappa}^{(d)}(\cdot\,,\cdot\ t)$ is explicitly known and it is given by the Mehler's formula, see (A.3)-(A.4). It is derived from (1.4)-(1.6) and (1.5).

Next, it remains to estimate each one of the above quantity. For the quantity in (2.2):

Lemma 2.1. *$\forall d \in \{1, 2, 3\}$, $\forall L \in (0, \infty)$, $\forall \kappa > 0$ and $\forall t > 0$:*

$$\mathscr{Z}_{L,\kappa}^{(d)}(t) \leq \left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^{-d} \mathrm{e}^{-d\kappa\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}.$$

Proof of Lemma 2.1. Let $\beta > 0$ and $\kappa > 0$ be fixed. Due to (A.4), it is enough to treat only the case of $d = 1$. From (A.3) and by setting $x = y$, one has by direct computations:

$$\forall L \in (0, \infty),\, \forall t > 0, \quad \mathscr{Z}_{L,\kappa}^{(d=1)}(t) = \frac{\mathrm{erfc}\left(\sqrt{\kappa\tanh\left(\frac{\kappa}{2}t\right)}\,\frac{L}{2}\right)}{\sqrt{2\sinh(\kappa t)\tanh\left(\frac{\kappa}{2}t\right)}},$$

where erfc denotes the complementary error function, see e.g. [1, Eq. (7.1.2)]. From the Chernoff inequality which reads as: $\forall \alpha \geq 0$, $\mathrm{erfc}(\alpha) \leq \mathrm{e}^{-\alpha^2}$ along with the identity (B.5), one arrives at:

$$\forall L \in (0,\infty),\ \forall t > 0, \quad \mathscr{X}_{L,\kappa}^{(d=1)}(t) \leq \left(2 \sinh\left(\frac{\kappa}{2} t\right)\right)^{-1} \mathrm{e}^{-\kappa \frac{L^2}{4} \tanh\left(\frac{\kappa}{2} t\right)}. \qquad \square$$

As for the the quantity defined in (2.1), we establish the following estimates:

Proposition 2.2. *For any $d \in \{1,2,3\}$:*
(i). There exists a constant $C_d > 0$ and a $\mathcal{L} \geq 1$ s.t. $\forall L \in [\mathcal{L},\infty)$, $\forall \kappa > 0$ and $\forall t > 0$:

$$\left|\mathscr{Y}_{L,\kappa}^{(d)}(t)\right| \leq C_d (1+t)^{2d+\frac{3}{2}} \left\{(1+\sqrt{\kappa})^2 \left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^{-d} + \left(\frac{L}{\sqrt{t}}\right)^{d-1}\right\} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}. \tag{2.3}$$

(ii). There exists a constant $C_d > 0$ and $\forall 0 < \kappa_0 < 1$ there exists a $\mathcal{L}_{\kappa_0} > 0$ s.t. $\forall L \in [\mathcal{L}_{\kappa_0},\infty)$, $\forall \kappa \in [\kappa_0,\infty)$ and $\forall t > 0$:

$$\left|\mathscr{Y}_{L,\kappa}^{(d)}(t)\right| \leq C_d \left(1+\sqrt{\kappa}\right)(1+\kappa)^d (1+t)^{3(d+\frac{1}{2})} \left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^{-d} \mathrm{e}^{-\frac{\kappa}{32}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}. \tag{2.4}$$

By gathering Lemma 2.1 and Proposition 2.2 (*i*) (resp. (*ii*)) together, Theorem 1.1 (resp. Corollary 1.2) follows. The rest of this section is devoted to the proof of Proposition 2.2.

2.1 Proof of Proposition 2.2.

In view of (2.1), the first step consists in writing an expression for the difference between the two semigroup kernels. It is contained in the following lemma:

Lemma 2.3. *$\forall L \in (0,\infty)$, $\forall \kappa > 0$ and $\forall t > 0$:*

$$\forall (x,y) \in \Lambda_L^2, \quad G_{\infty,\kappa}^{(1)}(x,y;t) - G_{L,\kappa}^{(1)}(x,y;t) =$$
$$-\frac{1}{2}\int_0^t \mathrm{d}s \left\{G_{\infty,\kappa}^{(1)}(x,-\frac{L}{2};s)\left(\partial_z G_{L,\kappa}^{(1)}\right)(-\frac{L}{2},y;t-s) - G_{\infty,\kappa}^{(1)}(x,\frac{L}{2};s)\left(\partial_z G_{L,\kappa}^{(1)}\right)(\frac{L}{2},y;t-s)\right\}, \tag{2.5}$$

and in the case of $d = 2,3$, for any $(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$:

$$G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) - G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) = -\frac{1}{2}\int_0^t \mathrm{d}s \int_{\partial\Lambda_L^d} \mathrm{d}\sigma(\mathbf{z})\, G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{z};s)\left[\mathbf{n}_{\mathbf{z}} \cdot \nabla_{\mathbf{z}} G_{L,\kappa}^{(d)}(\mathbf{z},\mathbf{y};t-s)\right], \tag{2.6}$$

where $\mathrm{d}\sigma(\mathbf{z})$ denotes the measure on $\partial\Lambda_L^d$ and $\mathbf{n}_{\mathbf{z}}$ the outer normal to $\partial\Lambda_L^d$ at $\mathbf{z}$.

The proof of Lemma 2.3 in the case of $d = 3$ can be found in [5, Lem. 4.2], see also [6]. Since the generalization to $d = 1,2$ can be easily obtained by similar arguments, we do not give any proof.

Remind that the kernel $G_{\infty,\kappa}^{(d)}$ is explicitly known and given by the Mehler's formula. In view of (2.1) along with the expressions from Lemma 2.3, the actual problem comes down to deriving a sufficiently sharp estimate on the gradient of the finite-volume semigroup kernel allowing to bring out a gaussian decay in L for the quantity in (2.1). It is contained in the following proposition:

Proposition 2.4. *$\forall d \in \{1,2,3\}$:*
(i). There exists a constant $C_d > 0$ and $\mathcal{L} \geq 1$ s.t. $\forall L \in [\mathcal{L},\infty)$, $\forall \kappa > 0$, $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$|\nabla_{\mathbf{x}} G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)| \leq C_d \left\{\mathcal{P}_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) + \mathcal{R}_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\right\}, \tag{2.7}$$

$$\mathcal{P}_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) := (1+\sqrt{\kappa})(1+t)^{\frac{5}{2}}\sqrt{\coth\left(\frac{\kappa}{2}t\right)}\, G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,8); \tag{2.8}$$

$$\mathcal{R}_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) := \frac{(1+t)^{2d+1}}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};4t). \tag{2.9}$$

(ii). There exists a constant $C_d > 0$ and $\forall 0 < \kappa_0 < 1$ there exists a $\mathcal{L}_{\kappa_0} > 0$ s.t. $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$, $\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\left|\nabla_{\mathbf{x}} G_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t)\right| \leq C_d \left\{\mathcal{P}_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) + \hat{\mathcal{R}}_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t)\right\}, \tag{2.10}$$

$$\hat{\mathcal{R}}_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) := \kappa^{\frac{d}{2}}(1+\kappa)^{\frac{d}{2}} \frac{t^{\frac{d-1}{2}}}{(\sinh(\kappa t))^{\frac{d}{2}}}(1+t)^{\frac{5d}{2}+1} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)} G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{y}; 4t). \tag{2.11}$$

Here, $G_{\infty,\kappa}^{(d)}(\cdot\,,\cdot\,; t, \gamma)$, $\kappa > 0$ and $\gamma > 0$ is defined in (A.7) *and $G_{\infty,0}^{(d)}(\cdot\,,\cdot\,; t)$ in* (A.2)-(A.4).

Note that Proposition 2.4 contains in fact the key-estimates of this paper; its proof is placed in Sec. 2.2. We mention that the derivation of such estimates relies on a Duhamel-like formula for the finite-volume semigroup $G_{L,\kappa}(t)$, $L \in (0, \infty)$ obtained via a geometric perturbation theory.

Remark 2.5. A natural question arises: what is the difference between (2.9) and (2.11)? In (2.11), we artificially made appear the factor $(\sinh(\kappa t))^{\frac{d}{2}}$ in the denominator. The price to pay is that for $0 < \kappa < 1$, the estimate holds for L large enough chosen accordingly (i.e. $L \geq cste/\sqrt{\kappa}$).

Proof of Proposition 2.2. Denote $\varsigma_L = \pm L/2$. We begin with the assertion (i). Let us start with the case of $d = 1$. In view of (2.1), (2.5) and (2.7), we need to estimate $\forall L \in [\mathcal{L}, \infty)$:

$$\forall t > 0, \quad \mathcal{Y}_{L,\kappa}^{(d=1),1}(t) := \frac{1}{2}\int_0^t \mathrm{d}s \int_{\Lambda_L^1} \mathrm{d}x\, G_{\infty,\kappa}^{(d=1)}(x, \varsigma_L; s, 1) \mathcal{P}_{\infty,\kappa}^{(d=1)}(\varsigma_L, x; t-s), \tag{2.12}$$

$$\mathcal{Y}_{L,\kappa}^{(d=1),2}(t) := \frac{1}{2}\int_0^t \mathrm{d}s \int_{\Lambda_L^1} \mathrm{d}x\, G_{\infty,\kappa}^{(d=1)}(x, \varsigma_L; s, 1) \mathcal{R}_{L,\kappa}^{(d=1)}(\varsigma_L, x; t-s). \tag{2.13}$$

Here, we have commuted the two integrals; this will be justified by what follows. We first estimate the quantity in (2.12). In view of (A.3) and (2.8), then from (A.14) for any $L \in [\mathcal{L}, \infty)$ and $t > 0$:

$$\mathcal{Y}_{L,\kappa}^{(d=1),1}(t) \leq C\sqrt{\kappa}\left(1+\sqrt{\kappa}\right)(1+t)^{\frac{5}{2}} \frac{1}{\sqrt{2\sinh(\kappa t)}} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)} \int_0^t \mathrm{d}s \sqrt{\coth\left(\frac{\kappa}{2}(t-s)\right)}, \tag{2.14}$$

for some constant $C > 0$. By using the upper bound in (B.4) along with the inequality:

$$\frac{1}{\sqrt{2\sinh(\kappa t)}} = \frac{\sqrt{\tanh\left(\frac{\kappa}{2}t\right)}}{\sqrt{2\sinh(\kappa t)\tanh\left(\frac{\kappa}{2}t\right)}} = \frac{\sqrt{\tanh\left(\frac{\kappa}{2}t\right)}}{2\sinh\left(\frac{\kappa}{2}t\right)} \leq \frac{1}{2\sinh\left(\frac{\kappa}{2}t\right)}, \tag{2.15}$$

justified by (B.5), then there exists another constant $C > 0$ s.t. $\forall L \in [\mathcal{L}, \infty)$ and $\forall t > 0$:

$$\mathcal{Y}_{L,\kappa}^{(d=1),1}(t) \leq C\left(1+\sqrt{\kappa}\right)\sqrt{1+\kappa} \frac{(1+t)^{\frac{7}{2}}}{2\sinh\left(\frac{\kappa}{2}t\right)} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}. \tag{2.16}$$

Next, let us estimate the quantity in (2.13). In view of (2.9) and (A.3), $\forall L \in [\mathcal{L}, \infty)$ and $\forall t > 0$:

$$\mathcal{Y}_{L,\kappa}^{(d=1),2}(t) \leq (1+t)^3 \int_0^t \frac{\mathrm{d}s}{\sqrt{t-s}} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)} \int_{\Lambda_L^1} \mathrm{d}x\, G_{\infty,\kappa}^{(d=1)}(x, \varsigma_L; s, 1) G_{\infty,0}^{(d=1)}(\varsigma_L, x; 4(t-s)).$$

Now, we want to make appear from the integration over Λ_L^1 a Gaussian decay in L while having the argument s. To do so, let us remark that on $\mathbb{R}^{2d}$, $d \in \{1, 2, 3\}$ one has for any $s > 0$:

$$G_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; s, 1) \leq \mathrm{e}^{-\frac{\kappa}{4}\left(|\mathbf{x}|^2+|\mathbf{y}|^2\right)\tanh\left(\frac{\kappa}{2}s\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; s, 2). \tag{2.17}$$

To get (2.17), we expanded in (A.3) the squares and used that $2ab \leq (a^2 + b^2)$, combined with the fact that $\coth(\alpha) - \tanh(\alpha) \geq 0$ $\forall \alpha > 0$. From (2.17) and (B.9), then by using the upper bound in the second inequality of (A.8) along with (A.13), one arrives $\forall L \in [\mathcal{L}, \infty)$ and $\forall t > 0$ at:

$$\mathcal{Y}_{L,\kappa}^{(d=1),2}(t) \leq C\frac{(1+t)^3}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)} \int_0^t \frac{\mathrm{d}s}{\sqrt{t-s}}, \tag{2.18}$$

for some constant $C > 0$. Gathering (2.16)-(2.18) together, we obtain (2.3) in the case of $d = 1$. Let us turn to the case of $d = 2$. The quantity in (2.6) being made up of four terms, then the same holds for the quantity in (2.1). Since these terms have exactly the same structure, it is enough to treat only one of them. In view of (2.7), we need to estimate $\forall L \in [\mathcal{L}, \infty)$ and $\forall t > 0$:

$$\mathcal{Y}_{L,\kappa}^{(d=2),1}(t) := \frac{1}{2} \int_0^t \mathrm{d}s \int_{\Lambda_L^2} \mathrm{d}\mathbf{x} \int_{\Lambda_L^1} \mathrm{d}z_1\, G_{\infty,\kappa}^{(d=2)}(\mathbf{x}, (z_1, \varsigma_L); s, 1) \mathcal{P}_{\infty,\kappa}^{(d=2)}((z_1, \varsigma_L), \mathbf{x}; t-s), \tag{2.19}$$

$$\mathcal{Y}_{L,\kappa}^{(d=2),2}(t) := \frac{1}{2} \int_0^t \mathrm{d}s \int_{\Lambda_L^2} \mathrm{d}\mathbf{x} \int_{\Lambda_L^1} \mathrm{d}z_1\, G_{\infty,\kappa}^{(d=2)}(\mathbf{x}, (z_1, \varsigma_L); s, 1) \mathcal{R}_{L,\kappa}^{(d=2)}((z_1, \varsigma_L), \mathbf{x}; t-s). \tag{2.20}$$

The strategy consists in using the property (A.4) in order to use the results stated in the case of $d = 1$. Let us first estimate the quantity in (2.19). In view of (A.4) and (2.8), then from (A.14):

$$\int_{\Lambda_L^2} \mathrm{d}\mathbf{x} \int_{\Lambda_L^1} \mathrm{d}z_1\, G_{\infty,\kappa}^{(d=2)}(\mathbf{x}, (z_1, \varsigma_L); s, 1) G_{\infty,\kappa}^{(d=2)}((z_1, \varsigma_L), \mathbf{x}; t-s, 8)$$
$$\leq C \int_{\mathbb{R}^1} \mathrm{d}x_1\, G_{\infty,\kappa}^{(d=1)}(x_1, x_1; t, 8) \int_{\mathbb{R}^1} \mathrm{d}x_2\, G_{\infty,\kappa}^{(d=1)}(x_2, \varsigma_L; s, 1) G_{\infty,\kappa}^{(d=1)}(\varsigma_L, x_2; t-s, 8),$$

for some constant $C > 0$. From (A.18), the first integral in the above r.h.s. is nothing but the trace (multiplied by a constant). Then, for any $L \in [\mathcal{L}, \infty)$ and $t > 0$, we arrive at:

$$\mathcal{Y}_{L,\kappa}^{(d=2),1}(t) \leq C \left(1 + \sqrt{\kappa}\right) \frac{(1+t)^{\frac{5}{2}}}{2 \sinh\left(\frac{\kappa}{2} t\right)}$$
$$\times \int_0^t \mathrm{d}s \sqrt{\coth\left(\frac{\kappa}{2}(t-s)\right)} \int_{\mathbb{R}^1} \mathrm{d}x_2\, G_{\infty,\kappa}^{(d=1)}(x_2, \varsigma_L; s, 1) G_{\infty,\kappa}^{(d=1)}(\varsigma_L, x_2; t-s, 8),$$

for another constant $C > 0$. The integral w.r.t. s has been estimated in the case of $d = 1$, see (2.14). Then it remains to mimic the arguments leading to (2.16) to conclude. Next, we estimate the quantity in (2.20). In view of (A.3)-(A.4) and (2.9), then from (A.8) followed by (A.14):

$$\int_{\Lambda_L^2} \mathrm{d}\mathbf{x} \int_{\Lambda_L^1} \mathrm{d}z_1\, G_{\infty,\kappa}^{(d=2)}(\mathbf{x}, (z_1, \varsigma_L); s, 1) G_{\infty,0}^{(d=2)}((z_1, \varsigma_L), \mathbf{x}; 4(t-s))$$
$$\leq C \int_{\Lambda_L^1} \mathrm{d}x_1\, G_{\infty,0}^{(d=1)}(x_1, x_1; 4t) \int_{\mathbb{R}^1} \mathrm{d}x_2\, G_{\infty,\kappa}^{(d=1)}(x_2, \varsigma_L; s, 1) G_{\infty,0}^{(d=1)}(\varsigma_L, x_2; 4(t-s)),$$

for some constant $C > 0$. Since the integrand in the first integral is nothing but a constant, this will make appear a factor L. Hence, in view of (2.9) and (A.3), one has $\forall L \in [\mathcal{L}, \infty)$ and $\forall t > 0$:

$$\mathcal{Y}_{L,\kappa}^{(d=2),2}(t) \leq CL \frac{(1+t)^5}{\sqrt{t}} \int_0^t \frac{\mathrm{d}s}{\sqrt{t-s}}\, \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)}$$
$$\times \int_{\mathbb{R}^1} \mathrm{d}x_2\, G_{\infty,\kappa}^{(d=1)}(x_2, \varsigma_L; s, 1) G_{\infty,0}^{(d=1)}(\varsigma_L, x_2; 4(t-s)),$$

for another $C > 0$. The integral w.r.t. s has been estimated in the case of $d = 1$. It remains to mimic the arguments leading to (2.18) to conclude. The case of $d = 3$ follows by similar arguments.

Subsequently, we prove the assertion (ii). Let $\kappa_0 > 0$ be fixed. Let us start with the case of $d = 1$. In view of (2.10), we only need to estimate $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$ the quantity:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=1),2}(t) := \frac{1}{2} \int_0^t \mathrm{d}s \int_{\Lambda_L^1} \mathrm{d}x\, G_{\infty,\kappa}^{(d=1)}(x, \varsigma_L; s, 1) \hat{\mathcal{R}}_{L,\kappa}^{(d=1)}(\varsigma_L, x; t-s).$$

From (2.11) and (A.3), one has $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$ and $\forall t > 0$:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=1),2}(t) \leq \sqrt{\kappa}\sqrt{1+\kappa}(1+t)^{\frac{7}{2}} \int_0^t \frac{\mathrm{d}s}{\sqrt{\sinh(\kappa(t-s))}} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)} \\ \times \int_{\Lambda_L^1} \mathrm{d}x\, G_{\infty,\kappa}^{(d=1)}(x, \varsigma_L; s, 1) G_{\infty,0}^{(d=1)}(\varsigma_L, x; 4(t-s)).$$

Now, from (2.17) followed by (B.9), then by using the upper bound in the first inequality of (A.8) along with (A.13), one has $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$ and $\forall t > 0$:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=1),2}(t) \leq C\kappa\sqrt{1+\kappa}\frac{(1+t)^{\frac{7}{2}}}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)} \int_0^t \mathrm{d}s\, \frac{\sqrt{s}}{\sqrt{\sinh(\kappa s)\sinh(\kappa(t-s))}},$$

for some $C > 0$. It remains to use successively (B.7), (B.4) and (2.15) which lead together to:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=1),2}(t) \leq C\sqrt{\kappa}(1+\kappa)\sqrt{t}\frac{(1+t)^4}{2\sinh\left(\frac{\kappa}{2}t\right)} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}, \tag{2.21}$$

for another constant $C > 0$. Gathering (2.16)-(2.21) together, we get (2.4) in the case of $d = 1$. Let us turn to the case of $d = 2$. In view of (2.10), we only need to estimate $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=2),2}(t) := \frac{1}{2}\int_0^t \mathrm{d}s \int_{\Lambda_L^2} \mathrm{d}\mathbf{x} \int_{\Lambda_L^1} \mathrm{d}z_1\, G_{\infty,\kappa}^{(d=2)}(\mathbf{x}, (z_1, \varsigma_L); s, 1) \hat{\mathcal{R}}_{L,\kappa}^{(d=2)}((z_1, \varsigma_L), \mathbf{x}; t-s).$$

In view of (A.3)-(A.4) and (2.11), then from the first upper bound in (A.8) followed by (A.14):

$$\int_{\Lambda_L^2} \mathrm{d}\mathbf{x} \int_{\Lambda_L^1} \mathrm{d}z_1\, G_{\infty,\kappa}^{(d=2)}(\mathbf{x}, (z_1, \varsigma_L); s, 1) G_{\infty,0}^{(d=2)}((z_1, \varsigma_L), \mathbf{x}; 4(t-s)) \leq C\sqrt{\frac{\kappa}{\sinh(\kappa s)}}\sqrt{s} \\ \times \int_{\Lambda_L^1} \mathrm{d}x_1\, G_{\infty,0}^{(d=1)}(x_1, x_1; 4t) \int_{\mathbb{R}^1} \mathrm{d}x_2\, G_{\infty,\kappa}^{(d=1)}(x_2, \varsigma_L; s, 1) G_{\infty,0}^{(d=1)}(\varsigma_L, x_2; 4(t-s)),$$

for some constant $C > 0$. Note that the integrand in the first integral of the above r.h.s. is nothing but a constant. This will make appear a factor L, but we will get rid of it at the end. Ergo, in view of (2.11) and (A.3), there exists another $C > 0$ s.t. $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$ and $\forall t > 0$:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=2),2}(t) \leq C\kappa^{\frac{3}{2}}(1+\kappa)L\frac{(1+t)^6}{\sqrt{t}} \int_0^t \mathrm{d}s\, \frac{\sqrt{s}\sqrt{t-s}}{\sqrt{\sinh(\kappa s)}\sinh(\kappa(t-s))} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)} \\ \times \int_{\mathbb{R}^1} \mathrm{d}x_2\, G_{\infty,\kappa}^{(d=1)}(x_2, \varsigma_L; s, 1) G_{\infty,0}^{(d=1)}(\varsigma_L, x_2; 4(t-s)).$$

The rest of the proof mimics the strategy we used for the case of $d = 1$. By using the upper bound in the first inequality of (A.8) along with (A.13), one has $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$ and $\forall t > 0$:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=2),2}(t) \leq C\kappa^2(1+\kappa)L\frac{(1+t)^6}{t} \int_0^t \mathrm{d}s\, \frac{s\sqrt{t-s}}{\sinh(\kappa s)\sinh(\kappa(t-s))} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)} \mathrm{e}^{-\frac{\kappa}{4}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}s\right)}.$$

Using successively (B.9), (B.7) and (2.50) leads to:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=2),2}(t) \leq C\kappa(1+\kappa)^2 L\sqrt{t}\frac{(1+t)^7}{2\sinh(\kappa t)} \mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)},$$

for another L-independent $C > 0$. It remains to use (A.16) to get rid of the L-factor:

$$\frac{L}{2\sinh(\kappa t)} \mathrm{e}^{-\frac{\kappa}{32}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)} \leq \frac{C}{\sqrt{\kappa}} \frac{1}{2\sinh(\kappa t)\sqrt{\tanh\left(\frac{\kappa}{2}t\right)}} \leq \frac{C}{\sqrt{\kappa}} \frac{1}{\left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^2}.$$

Gathering the above estimates together, one arrives $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$ and $\forall t > 0$ at:

$$\hat{\mathcal{Y}}_{L,\kappa}^{(d=2),2}(t) \leq C\sqrt{\kappa}(1+\kappa)^2\sqrt{t}\frac{(1+t)^7}{\left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^2}\mathrm{e}^{-\frac{\kappa}{32}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)},$$

for another constant $C > 0$. The case of $d = 3$ can be deduced by similar arguments. □

2.2 Proof of Proposition 2.4.

As previously mentioned, Proposition 2.4 contains the key-estimates to prove Theorem 1.1 and Corollary 1.2. The proof heavily leans on an approximation of the finite-volume semigroup operator via a geometric perturbation theory. For further applications, see [9] and also [10, 17].

2.2.1 An approximation via a geometric perturbation theory.

The key-idea consists in isolating in Λ_L^d the region close to the boundary from the bulk where the semigroup $G_{\infty,\kappa}(t)$ will act. The underlying difficulty is to keep a good control of the remainder terms arising from this approximation. This will be achieved by using well-chosen cutoff functions.

For any $0 < \eta < 1$, $0 < \vartheta \leq 1000$, $d \in \{1, 2, 3\}$ and $L \in (0, \infty)$ define:

$$\Theta_{L,\eta}(\vartheta) := \left\{\mathbf{x} \in \overline{\Lambda_L^d} : \mathrm{dist}\left(\mathbf{x}, \partial\Lambda_L^d\right) \leq \vartheta L^\eta\right\}. \tag{2.22}$$

For L sufficiently large, $\Theta_{L,\eta}(\vartheta)$ models a 'thin' compact subset of Λ_L^d near the boundary with Lebesgue-measure $|\Theta_{L,\eta}(\vartheta)|$ of order $\mathcal{O}(L^{(d-1)+\eta})$. For any $0 < \eta < 1$, let $L_0 = L_0(\eta) \geq 1$ s.t.

$$\Theta_{L_0,\eta}(1000) \subsetneq \Lambda_{L_0}^d, \quad L_0 - L_0^\eta \geq L_0/\sqrt{2}, \tag{2.23}$$

and L_0 large enough. Let us now introduce some well-chosen families of smooth cutoff functions. Let $f_{L,\eta}$ and $f_{L,\eta}^c$, $L \in [L_0(\eta), \infty)$ be a partition of the unity of Λ_L^d satisfying:

$$f_{L,\eta} + f_{L,\eta}^c = 1 \quad \text{on } \Lambda_L^d;$$

$$\mathrm{Supp}\,(f_{L,\eta}) \subset \left(\Lambda_L^d \setminus \Theta_{L,\eta}\left(\frac{1}{16}\right)\right), \quad f_{L,\eta} = 1 \text{ if } \mathbf{x} \in \left(\Lambda_L^d \setminus \Theta_{L,\eta}\left(\frac{1}{8}\right)\right), \quad 0 \leq f_{L,\eta} \leq 1;$$

$$\mathrm{Supp}\,(f_{L,\eta}^c) \subset \Theta_{L,\eta}\left(\frac{1}{8}\right), \quad f_{L,\eta}^c = 1 \text{ if } \mathbf{x} \in \Theta_{L,\eta}\left(\frac{1}{16}\right).$$

Moreover, there exists a constant $C > 0$ s.t.

$$\forall L \geq L_0(\eta), \quad \|D^\sigma f_{L,\eta}\|_\infty \leq CL^{-|\sigma|\eta}, \quad \forall |\sigma| \leq 2,\ |\sigma| = \sigma_1 + \cdots + \sigma_d.$$

Also, let $\hat{f}_{L,\eta}$ and $\hat{\hat{f}}_{L,\eta}$, $L \in [L_0(\eta), \infty)$ satisfying:

$$\mathrm{Supp}\left(\hat{f}_{L,\eta}\right) \subset \left(\Lambda_L^d \setminus \Theta_{L,\eta}\left(\frac{1}{64}\right)\right), \quad \hat{f}_{L,\eta} = 1 \text{ if } \mathbf{x} \in \left(\Lambda_L^d \setminus \Theta_{L,\eta}\left(\frac{1}{32}\right)\right), \quad 0 \leq \hat{f}_{L,\eta} \leq 1;$$

$$\mathrm{Supp}\left(\hat{\hat{f}}_{L,\eta}\right) \subset \Theta_{L,\eta}\left(\frac{1}{2}\right), \quad \hat{\hat{f}}_{L,\eta} = 1 \text{ if } \mathbf{x} \in \Theta_{L,\eta}\left(\frac{1}{4}\right), \quad 0 \leq \hat{\hat{f}}_{L,\eta} \leq 1.$$

Moreover, there exists another constant $C > 0$ s.t.

$$\forall L \geq L_0(\eta), \quad \max\left\{\left\|D^\sigma \hat{f}_{L,\eta}\right\|_\infty, \left\|D^\sigma \hat{\hat{f}}_{L,\eta}\right\|_\infty\right\} \leq CL^{-|\sigma|\eta}, \quad \forall |\sigma| \leq 2.$$

With these properties, one straightforwardly gets:

$$\hat{f}_{L,\eta} f_{L,\eta} = f_{L,\eta}; \tag{2.24}$$

$$\mathrm{dist}\left(\mathrm{Supp}\left(D^\sigma \hat{f}_{L,\eta}\right), \mathrm{Supp}\left(D^\tau f_{L,\eta}\right)\right) \geq CL^\eta, \quad \forall 1 \leq |\sigma| \leq 2,\ \forall 0 \leq |\tau| \leq 2; \tag{2.25}$$

$$\hat{\hat{f}}_{L,\eta} f_{L,\eta}^c = f_{L,\eta}^c; \tag{2.26}$$

$$\mathrm{dist}\left(\mathrm{Supp}\left(D^\sigma \hat{\hat{f}}_{L,\eta}\right), \mathrm{Supp}\left(D^\tau f_{L,\eta}^c\right)\right) \geq CL^\eta, \quad \forall 1 \leq |\sigma| \leq 2,\ \forall 0 \leq |\tau| \leq 2, \tag{2.27}$$

for some L-independent constants $C > 0$.

Afterwards, let us define $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$ (see (2.23)) and $\forall \kappa > 0$ on $\mathcal{C}_0^\infty(\Lambda_L^d)$:

$$h_{L,\kappa,\eta} := \frac{1}{2}\left(-i\nabla_{\mathbf{x}}\right)^2 + \frac{1}{2}\kappa^2 V_{L,\eta}(\mathbf{x}), \quad V_{L,\eta}(\mathbf{x}) := \begin{cases} |\mathbf{x}|^2, & \text{if } \mathbf{x} \in \mathrm{Supp}\left(\hat{\hat{f}}_{L,\eta}\right), \\ \frac{1}{4}\left(L - L^\eta\right)^2, & \text{otherwise.} \end{cases} \tag{2.28}$$

By standard arguments, (2.28) extends to a family of self-adjoint and semi-bounded operators for any $L \in [L_0(\eta), \infty)$, denoted again by $h_{L,\kappa,\eta}$, with domain $D(h_{L,\kappa,\eta}) = W_0^{1,2}(\Lambda_L^d) \cap W^{2,2}(\Lambda_L^d)$. $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$ and $\forall \kappa > 0$, let $\{g_{L,\kappa,\eta}(t) := \mathrm{e}^{-t h_{L,\kappa,\eta}} : L^2(\Lambda_L^d) \to L^2(\Lambda_L^d)\}_{t \geq 0}$ be the strongly-continuous one-parameter semigroup generated by $h_{L,\kappa,\eta}$. It is an integral operator with an integral kernel jointly continuous in $(\mathbf{x}, \mathbf{y}, t) \in \overline{\Lambda_L^d} \times \overline{\Lambda_L^d} \times (0, \infty)$. We denote it by $g_{L,\kappa,\eta}^{(d)}$.

Next, introduce $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$ and $\forall \kappa > 0$ the following operators on $L^2(\Lambda_L^d)$:

$$\forall t > 0, \quad \mathcal{G}_{L,\kappa,\eta}(t) := \hat{f}_{L,\eta} G_{\infty,\kappa}(t) f_{L,\eta} + \hat{\hat{f}}_{L,\eta} g_{L,\kappa,\eta}(t) f_{L,\eta}^c, \tag{2.29}$$

$$\begin{aligned} \mathcal{W}_{L,\kappa,\eta}(t) := &- \left\{\frac{1}{2}\left(\Delta \hat{f}_{L,\eta}\right) + i\left(\nabla \hat{f}_{L,\eta}\right) \cdot (-i\nabla)\right\} G_{\infty,\kappa}(t) f_{L,\eta} + \\ &- \left\{\frac{1}{2}\left(\Delta \hat{\hat{f}}_{L,\eta}\right) + i\left(\nabla \hat{\hat{f}}_{L,\eta}\right) \cdot (-i\nabla)\right\} g_{L,\kappa,\eta}(t) f_{L,\eta}^c. \end{aligned} \tag{2.30}$$

Sometimes, we will use the shorthand notations:

$$\forall t > 0, \quad \mathcal{G}_{L,\kappa,\eta}^{(p)}(t) := \hat{f}_{L,\eta} G_{\infty,\kappa}(t) f_{L,\eta}, \quad \mathcal{G}_{L,\kappa,\eta}^{(r)}(t) := \hat{\hat{f}}_{L,\eta} g_{L,\kappa,\eta}(t) f_{L,\eta}^c. \tag{2.31}$$

The main result of this paragraph is the following Duhamel-like formula:

Proposition 2.6. *$\forall d \in \{1,2,3\}$, $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$ and $\forall \kappa > 0$, it takes place in the bounded operators sense on $L^2(\Lambda_L^d)$:*

$$\forall t > 0, \quad G_{L,\kappa}(t) = \mathcal{G}_{L,\kappa,\eta}(t) - \int_0^t \mathrm{d}s \, G_{L,\kappa}(t-s) \mathcal{W}_{L,\kappa,\eta}(s). \tag{2.32}$$

The proof of Proposition 2.6 can be found in Sec. 2.2.3; it is essentially based on the application of [8, Prop. 3] taking into account the features of the cutoff functions introduced previously.

Remark 2.7. One can derive the following upper bounds on the operator norms. $\forall d \in \{1,2,3\}$ there exist two constants $C_d, c > 0$ s.t. $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$, $\forall \kappa > 0$ and $\forall t > 0$:

$$\|\mathcal{G}_{L,\kappa,\eta}(t)\| \leq \left\|\mathcal{G}_{L,\kappa,\eta}^{(p)}(t)\right\| + \left\|\mathcal{G}_{L,\kappa,\eta}^{(r)}(t)\right\| \leq (\cosh(\kappa t))^{-\frac{d}{2}} + C_d \mathrm{e}^{-\frac{\kappa^2}{16} L^2 t}, \tag{2.33}$$

$$\|\mathcal{W}_{L,\kappa,\eta}(t)\| \leq C_d \sqrt{1+\kappa} \frac{\sqrt{1+t}}{\sqrt{t}} \mathrm{e}^{-c\frac{L^{2\eta}}{t}} \left\{1 + (1+t)^{d-\frac{1}{2}} \mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4} t}\right\}. \tag{2.34}$$

The upper bound (2.33) comes from (A.15) and (2.51). The rough estimate in (2.34) is derived from Lemmas 2.11 and A.1 along with the properties (2.25)-(2.27).

2.2.2 End of the proof.

The starting-point in the proof of Proposition 2.4 is the Duhamel-like formula in (2.32). Taking its adjoint, one has $\forall d \in \{1,2,3\}$, $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$ (see (2.23)) and $\forall \kappa > 0$ on $L^2(\Lambda_L^d)$:

$$\forall t > 0, \quad G_{L,\kappa}(t) = \mathcal{G}_{L,\kappa,\eta}^*(t) - \int_0^t \mathrm{d}s \, \mathcal{W}_{L,\kappa,\eta}^*(s) G_{L,\kappa}(t-s), \tag{2.35}$$

where the adjoint operator of $\mathcal{G}_{L,\kappa,\eta}(t)$ and $\mathcal{W}_{L,\kappa,\eta}(t)$ reads respectively as, see (2.29)-(2.30):

$$\mathcal{G}_{L,\kappa,\eta}^{*}(t) = f_{L,\eta} G_{\infty,\kappa}(t) \hat{f}_{L,\eta} + f_{L,\eta}^{c} g_{L,\kappa,\eta}(t) \hat{\hat{f}}_{L,\eta}, \tag{2.36}$$

$$\begin{aligned}\mathcal{W}_{L,\kappa,\eta}^{*}(t) = &-f_{L,\eta} G_{\infty,\kappa}(t) \frac{1}{2}\left(\Delta \hat{f}_{L,\eta}\right) + i f_{L,\eta}\left\{(-i\nabla) G_{\infty,\kappa}(t) - \left[(-i\nabla), G_{\infty,\kappa}(t)\right]\right\}\left(\nabla \hat{f}_{L,\eta}\right) + \\ &- f_{L,\eta}^{c} g_{L,\kappa,\eta}(t) \frac{1}{2}\left(\Delta \hat{\hat{f}}_{L,\eta}\right) + i f_{L,\eta}^{c}\left\{(-i\nabla) g_{L,\kappa,\eta}(t) - \left[(-i\nabla), g_{L,\kappa,\eta}(t)\right]\right\}\left(\nabla \hat{\hat{f}}_{L,\eta}\right).\end{aligned} \tag{2.37}$$

Here, $[\cdot\,,\cdot]$ denotes the usual commutator, and in the bounded operators sense:

$$\left[(-i\nabla), G_{\infty,\kappa}(t)\right] = -\int_0^t \mathrm{d}s\, G_{\infty,\kappa}(t-s)\left[(-i\nabla), H_{\infty,\kappa}\right] G_{\infty,\kappa}(s), \tag{2.38}$$

$$\left[(-i\nabla), g_{L,\kappa,\eta}(t)\right] = -\int_0^t \mathrm{d}s\, g_{L,\kappa,\eta}(t-s)\left[(-i\nabla), h_{L,\kappa,\eta}\right] g_{L,\kappa,\eta}(s). \tag{2.39}$$

Writing (2.35) in the kernels sense, it follows this identity which holds $\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\begin{aligned}&\nabla_{\mathbf{x}} G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) = \\ &\qquad \nabla_{\mathbf{x}}\left(\mathcal{G}_{L,\kappa,\eta}^{*}\right)^{(d)}(\mathbf{x},\mathbf{y};t) - \int_0^t \mathrm{d}s \int_{\Lambda_L^d} \mathrm{d}\mathbf{z}\, \nabla_{\mathbf{x}}\left(\mathcal{W}_{L,\kappa,\eta}^{*}\right)^{(d)}(\mathbf{x},\mathbf{z};s) G_{L,\kappa}^{(d)}(\mathbf{z},\mathbf{y};t-s).\end{aligned} \tag{2.40}$$

Next, we need the following lemma whose proof can be found in Sec. 2.2.4:

Lemma 2.8. *$\forall d \in \{1,2,3\}$ there exist two constants $c, C_d > 0$ s.t.:*
(i) *$\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$, $\forall \kappa > 0$, $\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:*

$$\left|\nabla_{\mathbf{x}}\left(\mathcal{G}_{L,\kappa,\eta}^{*}\right)^{(d)}(\mathbf{x},\mathbf{y};t)\right| \leq C_d\left\{P_{\infty,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) + R_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\right\},$$

$$P_{\infty,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) := \left(1+\sqrt{\kappa}\right)\sqrt{\coth\left(\frac{\kappa}{2}t\right)}\, G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,2), \tag{2.41}$$

$$R_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) := \frac{(1+t)^d}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4}t} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t). \tag{2.42}$$

(ii). *$\forall \frac{1}{4} < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$, $\forall \kappa > 0$, $\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:*

$$\left|\nabla_{\mathbf{x}}\left(\mathcal{W}_{L,\kappa,\eta}^{*}\right)^{(d)}(\mathbf{x},\mathbf{y};t)\right| \leq C_d\left\{r_{\infty,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) + r_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\right\}, \tag{2.43}$$

$$r_{\infty,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) := \left(1+\sqrt{\kappa}\right)\sqrt{\coth\left(\frac{\kappa}{2}t\right)}(1+t)\mathrm{e}^{-c\kappa L^{2\eta}\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,8), \tag{2.44}$$

$$r_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) := \frac{(1+t)^{2d}}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}t} \mathrm{e}^{-c\frac{L^{2\eta}}{t}} \chi_{\Theta_{L,\eta}(\frac{1}{8})}(\mathbf{x}) G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};4t) \chi_{\Theta_{L,\eta}(\frac{1}{2})}(\mathbf{y}). \tag{2.45}$$

Here, $\chi_{\Theta_{L,\eta}(\vartheta)}$, $\vartheta > 0$ denotes the indicator function associated with $\Theta_{L,\eta}(\vartheta)$ defined in (2.22).

Remark 2.9. In (ii), the η has been restricted to $(\frac{1}{4}, 1)$ only to make the estimates more elegant.

Proof of Proposition 2.4. From now on, we set $\eta = \frac{1}{2}$ in the r.h.s. of (2.40). In view of the second term, (2.43) with (2.44)-(2.45) and (A.5), we need to estimate the two quantities:

$$\mathcal{Q}_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) := \int_0^t \mathrm{d}s \int_{\mathbb{R}^d} \mathrm{d}\mathbf{z}\, r_{\infty,\kappa,\eta=\frac{1}{2}}^{(d)}(\mathbf{x},\mathbf{z};s) G_{\infty,\kappa}^{(d)}(\mathbf{z},\mathbf{y};t-s,1), \tag{2.46}$$

$$\mathcal{Q}_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) := \int_0^t \mathrm{d}s \int_{\mathbb{R}^d} \mathrm{d}\mathbf{z}\, r_{L,\kappa,\eta=\frac{1}{2}}^{(d)}(\mathbf{x},\mathbf{z};s) G_{\infty,\kappa}^{(d)}(\mathbf{z},\mathbf{y};t-s,1). \tag{2.47}$$

Let $L \geq L_0(\eta = \frac{1}{2})$ defined in (2.23). We start with (2.46). From (2.44) followed by (A.14), there exist two constants $c, C > 0$ s.t. $\forall \kappa > 0$, $\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$Q_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) \leq C\left(1 + \sqrt{\kappa}\right)(1+t)\frac{\sqrt{\coth\left(\frac{\kappa}{2}t\right)}}{\sqrt{\coth\left(\frac{\kappa}{2}t\right)}} G_{\infty,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t, 8)\int_0^t \mathrm{d}s\, \sqrt{\coth\left(\frac{\kappa}{2}s\right)}\mathrm{e}^{-c\kappa L \coth\left(\frac{\kappa}{2}s\right)}.$$

By using (A.16) to get rid of the coth in the integrand, followed by the lower bound in (B.4) for the (artificial) denominator in the above r.h.s., then the upper bound in (2.8) follows. Let us turn to the quantity in (2.47). From (2.45), one has $\forall \kappa > 0$, $\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$Q_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) \leq (1+t)^{2d}\int_0^t \mathrm{d}s\, \frac{\mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}s}}{\sqrt{s}}\int_{\mathbb{R}^d}\mathrm{d}\mathbf{z}\, G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{z}; 4s)\chi_{\Theta_{L,\frac{1}{2}}(\frac{1}{2})}(\mathbf{z})G_{\infty,\kappa}^{(d)}(\mathbf{z}, \mathbf{y}; t-s, 1).$$

Now, we use (2.17) to make appear a Gaussian decay in L from the integration over $\mathbb{R}^d$. Here, the presence of the characteristic function in the integrand plays a crucial role. Since $\forall \mathbf{z} \in \Theta_{L,\frac{1}{2}}(\frac{1}{2})$, $|\mathbf{z}| \geq \frac{1}{2}(L - \sqrt{L})$ (remind that $L \geq L_0(\eta = \frac{1}{2})$, $L_0(\eta)$ as in (2.23)) then $\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\begin{aligned} Q_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) \leq (1+t)^{2d}\int_0^t \mathrm{d}s\, \frac{1}{\sqrt{s}}\mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}s}\mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)} \\ \times \int_{\Theta_{L,\eta}(\frac{1}{2})}\mathrm{d}\mathbf{z}\, G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{z}; 4s)G_{\infty,\kappa}^{(d)}(\mathbf{z}, \mathbf{y}; t-s, 2). \end{aligned} \quad (2.48)$$

Subsequently, we separate the proof of (i) from (ii). Extending the integration w.r.t. $\mathbf{z}$ to $\mathbb{R}^d$, then using successively the second upper bound in (A.8) and (A.13), (i) follows from the bound:

$$\mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}s}\mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)} \leq \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\left[\tanh\left(\frac{\kappa}{2}s\right)+\tanh\left(\frac{\kappa}{2}(t-s)\right)\right]} \leq \mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}, \quad 0 < s < t, \quad (2.49)$$

justified by the lower bound in (B.4) together with (B.9). Let us turn to (ii). Firstly, we extend the integration w.r.t. $\mathbf{z}$ to $\mathbb{R}^d$, then we use the first upper bound in (A.8) followed by (A.13). Secondly, we introduce a factor $s^{\frac{d-1}{2}}s^{-\frac{d-1}{2}}$ under the integral w.r.t s, and then we use successively the lower bound in (B.4) and the upper bound in (B.1) leading both to $(\kappa s)^{-\frac{d}{2}} \leq (\coth(\kappa s))^{\frac{d}{2}} \leq \mathrm{e}^{\frac{d}{2}\kappa s}(\sinh(\kappa s))^{-\frac{d}{2}}$. On this way, we get under the same conditions than (2.48):

$$Q_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) \leq C\kappa^d(1+t)^{2d}G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{y}; 4t)\int_0^t \mathrm{d}s\, \frac{s^{\frac{d-1}{2}}(t-s)^{\frac{d}{2}}\,\mathrm{e}^{\frac{d}{2}\kappa s}\mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}s}}{\{\sinh(\kappa s)\sinh(\kappa(t-s))\}^{\frac{d}{2}}}\mathrm{e}^{-\frac{\kappa}{8}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}(t-s)\right)},$$

for another constant $C > 0$. Here, we artificially made appear a $(\sinh(\kappa s))^{\frac{d}{2}}$ under the integration w.r.t. s. This leads to the appearance of a $\mathrm{e}^{\frac{d}{2}\kappa s}$ in the numerator. If $\kappa \geq 1$, we can get rid of it via the term $\mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}s}$ (for L large enough) since $\kappa \leq \kappa^2$. If $\kappa \in (0,1)$, one has to choose L large enough accordingly to κ (i.e. $L \geq cste/\sqrt{\kappa}$). Given a $\kappa_0 > 0$, let $\mathcal{L} = \mathcal{L}_{\kappa_0} \geq L_0(\frac{1}{2})$ s.t. $\forall L \geq \mathcal{L}_{\kappa_0}$, the inequality $\mathrm{e}^{-\frac{\kappa_0^2}{2}(\frac{1}{8}\frac{L^2}{4}-\frac{d}{\kappa_0})s} \leq \mathrm{e}^{-\frac{\kappa_0^2}{32}\frac{L^2}{4}s}$ holds. By using an inequality of type (2.49) followed by the identity in (B.7), then $\forall L \in [\mathcal{L}_{\kappa_0}, \infty)$, $\forall \kappa \in [\kappa_0, \infty)$, $\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$, we arrive at:

$$\begin{aligned} Q_{L,\kappa}^{(d)}(\mathbf{x}, \mathbf{y}; t) \leq C\kappa^d\frac{(1+t)^{2d}}{(\sinh(\kappa t))^{\frac{d}{2}}}\mathrm{e}^{-\frac{\kappa}{16}\frac{L^2}{4}\tanh\left(\frac{\kappa}{2}t\right)}G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{y}; 4t)\times \\ \times\int_0^t \mathrm{d}s\, s^{\frac{d-1}{2}}(t-s)^{\frac{d}{2}}\left\{(\coth(\kappa s))^{\frac{d}{2}} + (\coth(\kappa(t-s)))^{\frac{d}{2}}\right\}, \end{aligned}$$

for some constant $C > 0$. Here, we used that $(a+b)^\delta \leq 2^\delta(a^\delta + b^\delta)$ $\forall a, b, \delta > 0$. To conclude this estimate, it remains to use that there exists another constant $C > 0$ s.t. $\forall t > 0$ and $\forall \kappa > 0$:

$$\max\left\{\int_0^t \mathrm{d}s\, s^{\frac{d-1}{2}}(t-s)^{\frac{d}{2}}\left(\coth(\kappa s)\right)^{\frac{d}{2}}, \int_0^t \mathrm{d}s\, s^{\frac{d-1}{2}}(t-s)^{\frac{d}{2}}\left(\coth(\kappa(t-s))\right)^{\frac{d}{2}}\right\} \\ \leq C\frac{(1+\kappa)^{\frac{d}{2}}}{\kappa^{\frac{d}{2}}}(1+t)^{\frac{d}{2}}t^{\frac{d+1}{2}}. \quad (2.50)$$

To get (2.11), we have to modify the upper bound in (2.42) by mimicking the method used above to make appear the singularity $(\sinh(\kappa t))^{\frac{d}{2}}$ in the denominator (instead of $\sqrt{t}$). □

2.2.3 Proof of Proposition 2.6.

The proof leans on [8, Prop. 3] that we reproduce here for reader's convenience:

Proposition 2.10. *Let $\mathscr{H}$ be a separable Hilbert space and H be a self-adjoint and positive operator having the domain $D \subset \mathscr{H}$. Fix $t_0 > 0$. Assume that there exists an application $(0, t_0] \ni t \mapsto S(t) \in \mathfrak{B}(\mathscr{H})$ (the algebra of bounded operators on $\mathscr{H}$) with the following properties:* (A). $\sup_{0<t\leq t_0}\|S(t)\| \leq c_1 < \infty$. (B). *It is strongly differentiable,* $\mathrm{Ran}(S(t)) \subset D$ *and* $s-\lim_{t\downarrow 0} S(t) = \mathbb{1}$. (C). *There exists an application $(0, t_0] \ni t \mapsto R(t) \in \mathfrak{B}(\mathscr{H})$ continuous in the operator-norm sense s.t. $\|R(t)\| \leq c_2 t^{-\alpha}$ where $0 \leq \alpha < 1$, and:*

$$\frac{\partial S}{\partial t}(t)\phi + HS(t)\phi = R(t)\phi.$$

Then the following two statements are true:
(i). *The sequence of bounded operators ($n > [1/t]$):*

$$T_n(t) := \int_{\frac{1}{n}}^{t-\frac{1}{n}} \mathrm{d}s\, \exp[-(t-s)H]R(s),$$

converges in norm; let $T(t)$ be its limit;
(ii). *The following equality takes place on $\mathfrak{B}(\mathscr{H})$:* $\exp(-tH) = S(t) - T(t)$.

Before giving the proof, we need a series of estimates related with the kernel of the semigroup generated by the operator in (2.28). The proof of the below lemma can be found in Sec. 2.2.4.

Lemma 2.11. $\forall d \in \{1, 2, 3\}$ *there exists a constant $C_d > 0$ s.t. $\forall 0 < \eta < 1$, $\forall L \in [L_0(\eta), \infty)$, $\forall \kappa > 0$, $\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:*

$$g_{L,\kappa,\eta}^{(d)}(\mathbf{x}, \mathbf{y}; t) \leq C_d \mathrm{e}^{-\frac{\kappa^2}{4}\frac{L^2}{4}t} G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{y}; t), \quad (2.51)$$

$$\left|\nabla_{\mathbf{x}} g_{L,\kappa,\eta}^{(d)}(\mathbf{x}, \mathbf{y}; t)\right| \leq C_d \frac{(1+t)^d}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4}t} G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{y}; 2t), \quad (2.52)$$

$$\left|\Delta_{\mathbf{x}} g_{L,\kappa,\eta}^{(d)}(\mathbf{x}, \mathbf{y}; t)\right| \leq C_d \frac{(1+t)^{2d}}{t} \mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}t} G_{\infty,0}^{(d)}(\mathbf{x}, \mathbf{y}; 2t). \quad (2.53)$$

Proof of Proposition 2.6. The only thing we have to do is verify the assumptions of Proposition 2.10 in which $\mathcal{G}_{L,\kappa,\eta}(t)$ plays the role of $S(t)$. Let $0 < \eta < 1$, $L \in [L_0(\eta), \infty)$ and $\kappa > 0$ kept fixed. (A) From (2.33), $\mathcal{G}_{L,\kappa,\eta}(t)$ is uniformly bounded in t by some constant $C_d > 0$. (B) By using that $s - \lim_{t\downarrow 0} G_{\infty,\kappa}(t) = \mathbb{1}$ and $s - \lim_{t\downarrow 0} g_{L,\kappa,\eta}(t) = \mathbb{1}$ in the kernels sense, then:

$$\forall \phi \in L^2(\Lambda_L^d), \quad \lim_{t\downarrow 0} \mathcal{G}_{L,\kappa,\eta}\phi = \left\{\hat{f}_{L,\eta} f_{L,\eta} + \hat{\hat{f}}_{L,\eta} f_{L,\eta}^c\right\}\phi = \left\{f_{L,\eta} + f_{L,\eta}^c\right\}\phi = \phi,$$

where we used (2.24) and (2.26). Next, let us investigate the strong differentiability. From (2.31):

$$\forall \phi \in L^2(\Lambda_L^d), \quad \frac{1}{\delta t}\left\{\left(\mathcal{G}_{L,\kappa,\eta}^{(p)}(t+\delta t)\phi\right)(\cdot) - \left(\mathcal{G}_{L,\kappa,\eta}^{(p)}(t)\phi\right)(\cdot)\right\} \\ = \hat{f}_{L,\eta}(\cdot)\frac{1}{\delta t}\int_{\mathbb{R}^d} \mathrm{d}\mathbf{y}\left\{\int_{\mathbb{R}^d} \mathrm{d}\mathbf{z}\, G_{\infty,\kappa}^{(d)}(\cdot, \mathbf{z}; t) G_{\infty,\kappa}^{(d)}(\mathbf{z}, \mathbf{y}; \delta t) - G_{\infty,\kappa}^{(d)}(\cdot, \mathbf{y}; t)\right\} f_{L,\eta}(\mathbf{y})\phi(\mathbf{y}).$$

Since $G_{\infty,\kappa}(t)L^2(\mathbb{R}^d) \to D(H_{\infty,\kappa})$, then the Stone theorem (in the kernels sense) provides:

$$\lim_{\delta t \downarrow 0} \frac{1}{\delta t} \left\{ \left(\mathcal{G}_{L,\kappa,\eta}^{(p)}(t+\delta t)\phi \right)(\cdot) - \left(\mathcal{G}_{L,\kappa,\eta}^{(p)}(t)\phi \right)(\cdot) \right\} = -\hat{f}_{L,\eta}(\cdot) H_{\infty,\kappa} \int_{\mathbb{R}^d} \mathrm{d}\mathbf{y}\, G_{\infty,\kappa}^{(d)}(\cdot\,, \mathbf{y}; t) f_{L,\eta}(\mathbf{y})\phi(\mathbf{y}).$$

By using similar arguments to treat the contribution coming from $\mathcal{G}_{L,\kappa,\eta}^{(r)}(\cdot)$, we therefore obtain:

$$\lim_{\delta t \downarrow 0} \frac{1}{\delta t} \left\{ \mathcal{G}_{L,\kappa,\eta}(t+\delta t)\phi - \mathcal{G}_{L,\kappa,\eta}(t)\phi \right\} = -\hat{f}_{L,\eta} H_{\infty,\kappa} G_{\infty,\kappa}(t) f_{L,\eta}\phi - \hat{\hat{f}}_{L,\eta} h_{L,\kappa,\eta} g_{L,\kappa,\eta}(t) f_{L,\eta}^c \phi. \tag{2.54}$$

(C) Let $D_0 := \{\phi \in \mathcal{C}^1(\overline{\Lambda_L^d}) \cap \mathcal{C}^2(\Lambda_L^d), \phi|_{\partial \Lambda_L^d} = 0, \Delta\phi \in L^2(\Lambda_L^d)\}$ be the domain on which $H_{L,\kappa}$ is essentially self-adjoint. In the weak sense for any $\varphi \in D_0$, $\psi \in \mathcal{C}_0^\infty(\Lambda_L^d)$ and $t > 0$:

$$l_L(\varphi, \psi) := \langle H_{L,\kappa}\varphi, \mathcal{G}_{L,\kappa,\eta}(t)\psi \rangle_{L^2(\Lambda_L^d)} = -\left\langle \varphi, \frac{\partial \mathcal{G}_{L,\kappa,\eta}}{\partial t}(t)\psi \right\rangle_{L^2(\Lambda_L^d)} + \langle \varphi, \mathcal{W}_{L,\kappa,\eta}(t)\psi \rangle_{L^2(\Lambda_L^d)},$$

where $\frac{\partial \mathcal{G}_{L,\kappa,\eta}}{\partial t}(t)$ denotes the operator in the r.h.s. of (2.54). Note that the second equality is obtained by performing some integration by parts, and afterwards by using the following identities:

$$H_{L,\kappa}\hat{f}_{L,\eta} = H_{\infty,\kappa}\hat{f}_{L,\eta} = \left[H_{\infty,\kappa}, \hat{f}_{L,\eta} \right] + \hat{f}_{L,\eta} H_{\infty,\kappa},$$

as well as (remind that the potential V_L in (2.28) satisfies $V_L(\mathbf{x}) = |\mathbf{x}|^2$ on $\mathrm{Supp}(\hat{\hat{f}}_{L,\eta})$):

$$H_{L,\kappa}\hat{\hat{f}}_{L,\eta} = h_{L,\kappa,\eta}\hat{\hat{f}}_{L,\eta} = \left[h_{L,\kappa,\eta}, \hat{\hat{f}}_{L,\eta} \right] + \hat{\hat{f}}_{L,\eta} h_{L,\kappa,\eta}.$$

Since $l_L(\varphi, \cdot)$ is a bounded linear functional $\forall \varphi \in D_0$, then $\mathcal{C}_0^\infty(\Lambda_L^d) \ni \psi \mapsto l_L(\varphi, \psi)$ can be extended in a linear and bounded functional on $L^2(\Lambda_L^d)$ by the B.L.T. theorem. As well, since $l_L(\cdot\,, \psi)$ is a bounded linear functional $\forall \psi \in L^2(\Lambda_L^d)$ then $\varphi \mapsto l_L(\varphi, \psi)$ can be extended on the self-adjointness domain $D(H_{L,\kappa})$. This means that $\forall t > 0$, $\mathrm{Ran}(\mathcal{G}_{L,\kappa,\eta}(t)) \subset D(H_{L,\kappa})$. Hence:

$$\langle \varphi, H_{L,\kappa}\mathcal{G}_{L,\kappa,\eta}(t)\psi \rangle_{L^2(\Lambda_L^d)} = -\left\langle \varphi, \frac{\partial \mathcal{G}_{L,\kappa,\eta}}{\partial t}(t)\psi \right\rangle_{L^2(\Lambda_L^d)} + \langle \varphi, \mathcal{W}_{L,\kappa,\eta}(t)\psi \rangle_{L^2(\Lambda_L^d)}.$$

Finally, from (2.34) $\|\mathcal{W}_{L,\kappa,\eta}(t)\| \leq Ct^{-\frac{1}{2}}$ $\forall 0 < t \leq 1$. Hence $\|\mathcal{W}_{L,\kappa,\eta}(t)\|$ is integrable in $t \sim 0$. □

2.2.4 Proof of intermediary results.

Proof of Lemma 2.11. (2.51) follows from the Feynman-Kac formula in [14, Thm. X.68] together with (A.5) and the definition of the L_0 in (2.23) leading to $(L - L^\eta)^2 \geq L^2/2$ $\forall L \in [L_0(\eta), \infty)$. Next, let us turn to the proof of (2.52)-(2.53). To do that, let us introduce an operator of reference. $\forall d \in \{1,2,3\}$, $\forall 0 < \eta < 1$, $\forall L \in (0,\infty)$ and $\forall \kappa > 0$, define on $\mathcal{C}_0^\infty(\Lambda_L^d)$:

$$\tilde{h}_{L,\kappa,\eta} := \frac{1}{2}(-i\nabla_{\mathbf{x}})^2 + \frac{\kappa^2}{2}\tilde{V}_{L,\eta}(\mathbf{x}), \quad \tilde{V}_{L,\eta}(\mathbf{x}) := \frac{1}{4}(L - L^\eta)^2. \tag{2.55}$$

By standard arguments, (2.55) extends to a family of self-adjoint and semi-bounded operators for any $L \in (0,\infty)$, denoted again by $\tilde{h}_{L,\kappa,\eta}$. $\forall 0 < \eta < 1$, $\forall L \in (0,\infty)$ and $\forall \kappa > 0$, let $\{\tilde{g}_{L,\kappa,\eta}(t) := \mathrm{e}^{-t\tilde{h}_{L,\kappa,\eta}} : L^2(\Lambda_L^d) \to L^2(\Lambda_L^d)\}_{t \geq 0}$ be the strongly-continuous one-parameter semigroup generated by $\tilde{h}_{L,\kappa,\eta}$. Its integral kernel denoted by $\tilde{g}_{L,\kappa,\eta}^{(d)}$ is explicitly known and reads as:

$$\forall (\mathbf{x}, \mathbf{y}) \in \Lambda_L^{2d},\ \forall t > 0, \quad \tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x}, \mathbf{y}; t) = \mathrm{e}^{-\frac{\kappa^2}{8}(L - L^\eta)^2 t} G_{L,0}^{(d)}(\mathbf{x}, \mathbf{y}; t), \tag{2.56}$$

where $G_{L,0}^{(d)}$ is the kernel of the semigroup generated by the Dirichlet Laplacian in $L^2(\Lambda_L^d)$, see (A.6). Note that (2.56) directly follows from the Feynman-Kac formula. The starting-point of the proof of (2.52)-(2.53) is a Duhamel-like formula to express the semigroup $\{g_{L,\kappa,\eta}(t)\}_{t>0}$ in terms of $\{\tilde{g}_{L,\kappa,\eta}(t)\}_{t>0}$ whose integral kernel is given in (2.56). Let $0<\eta<1$, $L\in[L_0(\eta),\infty)$ (see (2.23)) and $\kappa>0$ be fixed. In the bounded operators sense on $L^2(\Lambda_L^d)$, it takes place:

$$\forall t>0,\quad g_{L,\kappa,\eta}(t)=\tilde{g}_{L,\kappa,\eta}(t)-\int_0^t \mathrm{d}s\,\tilde{g}_{L,\kappa,\eta}(s)\left\{h_{L,\kappa,\eta}-\tilde{h}_{L,\kappa,\eta}\right\}g_{L,\kappa,\eta}(t-s), \tag{2.57}$$

where we used the self-adjointness of the semigroups $\{g_{L,\kappa,\eta}(t)\}_{t\geq 0}$, $\{\tilde{g}_{L,\kappa,\eta}(t)\}_{t\geq 0}$.
Proof of (2.52). From (2.57), it follows in the kernels sense:

$$\forall(\mathbf{x},\mathbf{y})\in\Lambda_L^{2d},\ \forall t>0,\quad \nabla_{\mathbf{x}}g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)=\nabla_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)-\frac{1}{2}\mathfrak{q}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t), \tag{2.58}$$

$$\mathfrak{q}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t):=\kappa^2\int_0^t\mathrm{d}s\int_{\Lambda_L^d}\mathrm{d}\mathbf{z}\,\nabla_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{z};s)\left\{V_{L,\eta}(\mathbf{z})-\tilde{V}_{L,\eta}(\mathbf{z})\right\}g_{L,\kappa,\eta}^{(d)}(\mathbf{z},\mathbf{y};t-s).$$

Remind that $V_{L,\eta}(\mathbf{z})-\tilde{V}_{L,\eta}(\mathbf{z})=|\mathbf{z}|^2-\frac{1}{4}(L-L^\eta)^2$ on $\mathrm{Supp}(\hat{\hat{f}}_{L,\eta})$, 0 otherwise. Let us estimate the first kernel in the r.h.s. of (2.58). From (A.11) and (2.56), there exists a constant $C_d>0$ s.t.

$$\forall(\mathbf{x},\mathbf{y})\in\Lambda_L^{2d},\ \forall t>0,\quad \left|\nabla_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\right|\leq C_d\frac{(1+t)^d}{\sqrt{t}}\mathrm{e}^{-\frac{\kappa^2}{4}\frac{L^2}{4}t}G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t). \tag{2.59}$$

Subsequently, from (2.59) along with (2.51), there exists another constant $C_d>0$ s.t.

$$\forall(\mathbf{x},\mathbf{y})\in\Lambda_L^{2d},\ \forall t>0,\quad \left|\mathfrak{q}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\right|\leq C_d\kappa^2L^2(1+t)^d\mathrm{e}^{-\frac{\kappa^2}{4}\frac{L^2}{4}t}G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t)\int_0^t\frac{\mathrm{d}s}{\sqrt{s}},$$

where we used in the last inequality (A.13). Finally use (A.16) to get rid of the L^2 what leads to:

$$\left|\mathfrak{q}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\right|\leq C_d\frac{(1+t)^d}{\sqrt{t}}\mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4}t}G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t), \tag{2.60}$$

for another constant $C_d>0$. It remains to gather (2.59) and (2.60) together.
Proof of (2.53). Starting from the below identity which holds in the bounded operators sense:

$$\forall t>0,\quad [(-i\nabla),\tilde{g}_{L,\kappa,\eta}(t)]=-\int_0^t\mathrm{d}s\,\tilde{g}_{L,\kappa,\eta}(t-s)\left[(-i\nabla),\tilde{h}_{L,\kappa,\eta}\right]\tilde{g}_{L,\kappa,\eta}(s),$$

then by using that $[(-i\nabla),\tilde{h}_{L,\kappa,\eta}]=0$, one gets from (2.57) on $L^2(\Lambda_L^d)$:

$$\forall t>0,\quad (-i\nabla)\,g_{L,\kappa,\eta}(t)=(-i\nabla)\,\tilde{g}_{L,\kappa,\eta}(t)-\int_0^t\mathrm{d}s\,\tilde{g}_{L,\kappa,\eta}(s)\,(-i\nabla)\left\{h_{L,\kappa,\eta}-\tilde{h}_{L,\kappa,\eta}\right\}g_{L,\kappa,\eta}(t-s).$$

It follows in the kernels sense:

$$\forall(\mathbf{x},\mathbf{y})\in\Lambda_L^{2d},\forall t>0,\quad \Delta_{\mathbf{x}}g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)=\Delta_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)-\frac{1}{2}\sum_{l=1}^{2}\mathfrak{u}_{L,\kappa,\eta}^{(d),l}(\mathbf{x},\mathbf{y};t),$$

$$\mathfrak{u}_{L,\kappa,\eta}^{(d),1}(\mathbf{x},\mathbf{y};t):=\kappa^2\int_0^t\mathrm{d}s\int_{\Lambda_L^d}\mathrm{d}\mathbf{z}\,\nabla_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{z};s)\left(\nabla_{\mathbf{z}}V_{L,\eta}\right)(\mathbf{z})g_{L,\kappa,\eta}^{(d)}(\mathbf{z},\mathbf{y};t-s),$$

$$\mathfrak{u}_{L,\kappa,\eta}^{(d),2}(\mathbf{x},\mathbf{y};t):=\kappa^2\int_0^t\mathrm{d}s\int_{\Lambda_L^d}\mathrm{d}\mathbf{z}\,\nabla_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{z};s)\left\{\tilde{V}_{L,\eta}(\mathbf{z})-V_{L,\eta}(\mathbf{z})\right\}\nabla_{\mathbf{z}}g_{L,\kappa,\eta}^{(d)}(\mathbf{z},\mathbf{y};t-s).$$

From (A.12) and (2.56), there exists a constant $C_d>0$ s.t.

$$\forall(\mathbf{x},\mathbf{y})\in\Lambda_L^{2d},\forall t>0,\quad \left|\Delta_{\mathbf{x}}\tilde{g}_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\right|\leq C_d\frac{(1+t)^d}{t}\mathrm{e}^{-\frac{\kappa^2}{4}\frac{L^2}{4}t}G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t).$$

Subsequently, by mimicking the method leading to (2.60), there exists another $C_d > 0$ s.t.

$$\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d},\ \forall t > 0, \quad \left|\mathfrak{u}_{L,\kappa,\eta}^{(d),1}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \frac{(1+t)^d}{\sqrt{t}} \mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4}t} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t).$$

By the same method again, but replacing the estimate (2.51) with (2.52), we have:

$$\left|\mathfrak{u}_{L,\kappa,\eta}^{(d),2}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \frac{(1+t)^{2d}}{t} \mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}t} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t) \int_0^t \frac{\mathrm{d}s}{\sqrt{s}\sqrt{t-s}}.$$

Gathering the three above estimates together, then the proof of (2.53) is over. □

Proof of Lemma 2.8. Let $d \in \{1,2,3\}$, $0 < \eta < 1$, $L \in [L_0(\eta), \infty)$ and $\kappa > 0$ kept fixed.
(i). From (2.36) written in the kernels sense, then $\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\begin{aligned}\nabla_{\mathbf{x}} \left(\mathcal{G}_{L,\kappa,\eta}^{*}\right)^{(d)}(\mathbf{x},\mathbf{y};t) = \left(\nabla f_{L,\eta}\right)(\mathbf{x}) G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) \hat{f}_{L,\eta}(\mathbf{y}) + f_{L,\eta}(\mathbf{x}) \nabla_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) \hat{f}_{L,\eta}(\mathbf{y}) + \\ + \left(\nabla f_{L,\eta}^{c}\right)(\mathbf{x}) g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) \hat{\hat{f}}_{L,\eta}(\mathbf{y}) + f_{L,\eta}^{c}(\mathbf{x}) \nabla_{\mathbf{x}} g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t) \hat{\hat{f}}_{L,\eta}(\mathbf{y}).\end{aligned}$$

(2.41) is an upper bound for the two first kernels in the above r.h.s. obtained from (A.3)-(A.4) and (A.9). (2.42) is an upper bound for the two last kernels obtained from (2.51) and (2.52).
(ii). From (2.37) written in the kernels sense, then $\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\nabla_{\mathbf{x}} \left(\mathcal{W}_{L,\kappa,\eta}^{*}\right)^{(d)}(\mathbf{x},\mathbf{y};t) = \sum_{m=1}^{4} Q_{L,\kappa,\eta}^{(d),m}(\mathbf{x},\mathbf{y};t), \quad \text{with:}$$

$$\begin{aligned}Q_{L,\kappa,\eta}^{(d),1}(\mathbf{x},\mathbf{y};t) := -i\left(\nabla f_{L,\eta}\right)(\mathbf{x})\left[(-i\nabla), G_{\infty,\kappa}(t)\right](\mathbf{x},\mathbf{y})\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y}) + \\ + \left(\nabla f_{L,\eta}\right)(\mathbf{x}) \nabla_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y}) - \left(\nabla f_{L,\eta}\right)(\mathbf{x}) G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\frac{1}{2}\left(\Delta \hat{f}_{L,\eta}\right)(\mathbf{y}),\end{aligned} \tag{2.61}$$

$$\begin{aligned}Q_{L,\kappa,\eta}^{(d),2}(\mathbf{x},\mathbf{y};t) := -i f_{L,\eta}(\mathbf{x}) \nabla_{\mathbf{x}}\left[(-i\nabla), G_{\infty,\kappa}(t)\right](\mathbf{x},\mathbf{y})\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y}) + \\ + f_{L,\eta}(\mathbf{x}) \Delta_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y}) - f_{L,\eta}(\mathbf{x}) \nabla_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\frac{1}{2}\left(\Delta \hat{f}_{L,\eta}\right)(\mathbf{y}),\end{aligned} \tag{2.62}$$

$$\begin{aligned}Q_{L,\kappa,\eta}^{(d),3}(\mathbf{x},\mathbf{y};t) := -i\left(\nabla f_{L,\eta}^{c}\right)(\mathbf{x})\left[(-i\nabla), g_{L,\kappa,\eta}(t)\right](\mathbf{x},\mathbf{y})\left(\nabla \hat{\hat{f}}_{L,\eta}\right)(\mathbf{y}) + \\ + \left(\nabla f_{L,\eta}^{c}\right)(\mathbf{x}) \nabla_{\mathbf{x}} g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\left(\nabla \hat{\hat{f}}_{L,\eta}\right)(\mathbf{y}) - \left(\nabla f_{L,\eta}^{c}\right)(\mathbf{x}) g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\frac{1}{2}\left(\Delta \hat{\hat{f}}_{L,\eta}\right)(\mathbf{y}),\end{aligned} \tag{2.63}$$

$$\begin{aligned}Q_{L,\kappa,\eta}^{(d),4}(\mathbf{x},\mathbf{y};t) := -i f_{L,\eta}^{c}(\mathbf{x}) \nabla_{\mathbf{x}}\left[(-i\nabla), g_{L,\kappa,\eta}(t)\right](\mathbf{x},\mathbf{y})\left(\nabla \hat{\hat{f}}_{L,\eta}\right)(\mathbf{y}) + \\ + f_{L,\eta}^{c}(\mathbf{x}) \Delta_{\mathbf{x}} g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\left(\nabla \hat{\hat{f}}_{L,\eta}\right)(\mathbf{y}) - f_{L,\eta}^{c}(\mathbf{x}) \nabla_{\mathbf{x}} g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{y};t)\frac{1}{2}\left(\Delta \hat{\hat{f}}_{L,\eta}\right)(\mathbf{y}).\end{aligned} \tag{2.64}$$

Let us first estimate (2.61). In view of (A.9), (2.41) is clearly an upper bound for the two last terms in the r.h.s. of (2.61). For the first term in (2.61), we use (2.38) in the kernels sense. Then, there exists a constant $C_d > 0$ s.t. $\forall(\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\frac{\kappa^2}{2}\int_0^t \mathrm{d}s \int_{\mathbb{R}^d} \mathrm{d}\mathbf{z}\, G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{z};t-s)\left(\nabla_{\mathbf{z}}|\mathbf{z}|^2\right) G_{\infty,\kappa}^{(d)}(\mathbf{z},\mathbf{y};s) \leq C_d(\kappa^2 L + \kappa^{\frac{3}{2}}) t G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,2). \tag{2.65}$$

Here, we used that $|\mathbf{z}| \leq |\mathbf{x}-\mathbf{z}| + |\mathbf{x}|$, then (A.16) to get rid of the factor $|\mathbf{x}-\mathbf{z}|$ and (A.14), and finally the inequality $\coth(\alpha) \geq 1\ \forall \alpha > 0$. Now, we use the property (2.27) to get rid of the powers of κ in (2.65) via (A.16). Hence, there exist two other constants $c, C_d > 0$ s.t. on Λ_L^{2d}:

$$\begin{aligned}&\left|i\left(\nabla f_{L,\eta}\right)(\mathbf{x})\left[(-i\nabla), G_{\infty,\kappa}(t)\right](\mathbf{x},\mathbf{y})\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y})\right| \\ &\qquad \leq C_d L^{-3\eta}(1+L^{1-\eta}) t \mathrm{e}^{-c\kappa L^{2\eta}\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,4).\end{aligned}$$

Restricting to $1 > \eta > \frac{1}{4}$, and gathering the above estimate with (2.41) together, then there exist two other constants $c, C_d > 0$ s.t. $\forall L \in [L_0(\eta), \infty)$, $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\left|Q_{L,\kappa,\eta}^{(d),1}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \left(1+\sqrt{\kappa}\right)\sqrt{\coth\left(\frac{\kappa}{2}t\right)}(1+t)\mathrm{e}^{-c\kappa L^{2\eta}\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,4). \tag{2.66}$$

Subsequently, let us turn to (2.62). From (A.9) and (A.10) together with the property (2.25), then there exist two other constants $c, C_d > 0$ s.t. $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\begin{aligned}\Big|f_{L,\eta}(\mathbf{x})\nabla_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\frac{1}{2}\left(\Delta \hat{f}_{L,\eta}\right)(\mathbf{y}) + f_{L,\eta}(\mathbf{x})\Delta_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y})\Big| \\ \leq C_d\sqrt{\kappa}\sqrt{\coth\left(\frac{\kappa}{2}t\right)}\mathrm{e}^{-c\kappa L^{2\eta}\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,4).\end{aligned}$$

Here, the property (2.25) is essential to remove a $\sqrt{\coth(\kappa t)}$ in the numerator of (A.10). For the first term of (2.62), we use the same reasoning leading to (2.65) combined with the property (2.25). Thus, there exist two other constants $c, C_d > 0$ s.t. $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\begin{aligned}\frac{\kappa^2}{2}\left|f_{L,\eta}(\mathbf{x})\int_0^t \mathrm{d}s\int_{\mathbb{R}^d}\mathrm{d}\mathbf{z}\,\nabla_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{z};t-s)\left(\nabla_{\mathbf{z}}|\mathbf{z}|^2\right) G_{\infty,\kappa}^{(d)}(\mathbf{z},\mathbf{y};s)\left(\nabla \hat{f}_{L,\eta}\right)(\mathbf{y})\right| \\ \leq C_d\left(1+\sqrt{\kappa}\right)L^{-4\eta}(1+L)(1+t)\mathrm{e}^{-c\kappa L^{2\eta}\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,8).\end{aligned}$$

Restricting to $1 > \eta > \frac{1}{4}$, and gathering the above estimates together, then there exist two other constants $c, C_d > 0$ s.t. $\forall L \in [L_0(\eta), \infty)$, $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\left|Q_{L,\kappa,\eta}^{(d),2}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \left(1+\sqrt{\kappa}\right)\sqrt{\coth\left(\frac{\kappa}{2}t\right)}(1+t)\mathrm{e}^{-c\kappa L^{2\eta}\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,8). \tag{2.67}$$

The estimate in (2.44) follows by adding (2.66) and (2.67) together.
We continue with (2.63). (2.42) is an upper bound for the last two terms in the r.h.s. of (2.63). From (2.39) in the kernels sense, then by (A.16) there exist two other constants $c, C_d > 0$ s.t.

$$\frac{\kappa^2}{2}\int_0^t \mathrm{d}s\int_{\Lambda_L^d}\mathrm{d}\mathbf{z}\, g_{L,\kappa,\eta}^{(d)}(\mathbf{x},\mathbf{z};t-s)\left(\nabla_{\mathbf{z}} V_{L,\eta}\right)(\mathbf{z}) g_{L,\kappa,\eta}^{(d)}(\mathbf{z},\mathbf{y};s) \leq C_d \mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4}t}\mathrm{e}^{-c\frac{L^{2\eta}}{t}} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t).$$

We conclude that there exist two other constants $c, C_d > 0$ s.t. $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$:

$$\forall t > 0, \quad \left|Q_{L,\kappa,\eta}^{(d),3}(\mathbf{x},\mathbf{y};t)\right| \leq C_d\frac{(1+t)^d}{\sqrt{t}}\mathrm{e}^{-\frac{\kappa^2}{8}\frac{L^2}{4}t}\mathrm{e}^{-c\frac{L^{2\eta}}{t}} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};4t). \tag{2.68}$$

Concerning (2.64), one can prove that there exist two other constants $c, C_d > 0$ s.t. on Λ_L^{2d}:

$$\forall t > 0, \quad \left|Q_{L,\kappa,\eta}^{(d),4}(\mathbf{x},\mathbf{y};t)\right| \leq C_d\frac{(1+t)^{2d}}{\sqrt{t}}\mathrm{e}^{-\frac{\kappa^2}{16}\frac{L^2}{4}t}\mathrm{e}^{-c\frac{L^{2\eta}}{t}} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};4t). \tag{2.69}$$

Here, we used (2.27) combined with (A.16) to get rid of a $\sqrt{t}$ in the denominator of (2.53). The estimate in (2.45) follows by adding (2.68) and (2.69) together, then by taking into account the support of the cutoff functions introduced in Sec. 2.2.1. □

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A The semigroup: A review of some basic properties.

Here, we collect the technical results we use throughout the paper involving the semigroup generated by $H_{L,\kappa}$, see Sec. 1.1. For reader's convenience, all the proofs are placed in Sec. A.2.

A.1 Kernels, estimates and all these things.

For simplicity's sake, we use hereafter the notation $\Lambda_\infty := \mathbb{R}$. From (1.1)-(1.2), remind that:

$$\forall L \in (0,\infty], \quad H_{L,\kappa} = \frac{1}{2}(-i\nabla_{\mathbf{x}})^2 + \frac{1}{2}\kappa^2|\mathbf{x}|^2 \quad \text{in } L^2(\Lambda_L^d),\ d \in \{1,2,3\}. \tag{A.1}$$

Below, we allow the value $\kappa = 0$; in that case, $H_{L,0}$ with $L < \infty$ is nothing but the Dirichlet Laplacian and $H_{\infty,0}$ the free Laplacian on the whole space whose self-adjointness domain is $W^{2,2}(\Lambda_\infty^d)$.

Let us recall some properties on the strongly continuous one-parameter semigroup $\{G_{L,\kappa}(t) := \mathrm{e}^{-tH_{L,\kappa}} : L^2(\Lambda_L^d) \to L^2(\Lambda_L^d)\}_{t\geq 0}$ generated by $H_{L,\kappa}$ in (A.1). We refer to [18, Sec. B] and [20]. As already mentioned, $\forall \kappa \geq 0$ and $\forall L \in (0,\infty]$ it is a self-adjoint and positive operator on $L^2(\Lambda_L^d)$ by the spectral theorem and the functional calculus. Moreover, since $\{G_{L,\kappa}(t)\}_{t>0}$ is bounded from $L^2(\Lambda_L^d)$ to $L^\infty(\Lambda_L^d)$, then it is an integral operator by the Dunford-Gelf'and-Pettis theorem.

Let us turn to the integral kernel of $\{G_{L,\kappa}(t)\}_{t>0}$ we denote by $G_{L,\kappa}^{(d)}$. $\forall \kappa \geq 0$ and $\forall L \in (0,\infty]$, $G_{L,\kappa}^{(d)}$ is jointly continuous in $(\mathbf{x},\mathbf{y},t) \in \overline{\Lambda_L^d} \times \overline{\Lambda_L^d} \times (0,\infty)$ and vanishes if $\mathbf{x} \in \partial\Lambda_L^d$ or $\mathbf{y} \in \partial\Lambda_L^d$. When $L = \infty$, it is explicitly known. If $\kappa = 0$, it is the so-called heat kernel reading for $d = 1$ as:

$$\forall (x,y) \in \Lambda_\infty^2,\ \forall t > 0, \quad G_{\infty,0}^{(d=1)}(x,y;t) := \frac{1}{\sqrt{2\pi}} \frac{\mathrm{e}^{-\frac{(x-y)^2}{2t}}}{\sqrt{t}}. \tag{A.2}$$

If $\kappa > 0$, the one-dimensional kernel is given by the so-called Mehler's formula, see [12, pp. 176]:

$$\forall (x,y) \in \Lambda_\infty^2,\ \forall t > 0, \quad G_{\infty,\kappa}^{(d=1)}(x,y;t) = \sqrt{\frac{\kappa}{2\pi \sinh(\kappa t)}} \mathrm{e}^{-\frac{\kappa}{4}\left[(x+y)^2 \tanh\left(\frac{\kappa}{2}t\right) + (x-y)^2 \coth\left(\frac{\kappa}{2}t\right)\right]}. \tag{A.3}$$

Note that the multidimensional kernel (i.e. $d = 2,3$) is directly obtained from (A.2) or (A.3) by:

$$\forall \kappa \geq 0, \quad G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) := \prod_{j=1}^d G_{\infty,\kappa}^{(d=1)}(x_j,y_j;t), \quad \mathbf{x} := \{x_j\}_{j=1}^d,\ \mathbf{y} := \{y_j\}_{j=1}^d. \tag{A.4}$$

When restricting to $L \in (0,\infty)$, the mapping $L \mapsto G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)$ is positive and monotone increasing. This leads to the following pointwise inequality which holds $\forall \kappa \geq 0$ and $\forall L \in (0,\infty)$:

$$\forall (\mathbf{x},\mathbf{y},t) \in \overline{\Lambda_L^d} \times \overline{\Lambda_L^d} \times (0,\infty), \quad G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) \leq \sup_{L>0} G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t) = G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t). \tag{A.5}$$

We mention that, if $\kappa = 0$, the kernel $G_{L,0}^{(d)}$ is explicitly known and reads as, see [8, Eq. (4.13)]:

$$\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d},\ \forall t > 0, \quad G_{L,0}^{(d)}(\mathbf{x},\mathbf{y};t) = \prod_{j=1}^d G_{L,0}^{(d=1)}(x_j,y_j;t), \tag{A.6}$$

$$G_{L,0}^{(d=1)}(x,y;t) := \frac{1}{\sqrt{2t}} \sum_{m\in\mathbb{Z}} \left\{ \exp\left(-\frac{(x-y+2mL)^2}{2t}\right) - \exp\left(-\frac{(x+y-2mL-L)^2}{2t}\right) \right\}.$$

In view of (A.3)-(A.4), let us introduce $\forall \kappa > 0$ the new notation:

$$\forall \gamma > 0, \quad G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,\gamma) := \left(\frac{\kappa}{2\pi\sinh(\kappa t)}\right)^{\frac{d}{2}} \prod_{j=1}^d \mathrm{e}^{-\frac{\kappa}{4\gamma}\left[(x_j+y_j)^2 \tanh\left(\frac{\kappa}{2}t\right) + (x_j-y_j)^2 \coth\left(\frac{\kappa}{2}t\right)\right]}, \tag{A.7}$$

with the convention: $G_{\infty,\kappa}^{(d)}(\cdot\,,\cdot\,;t) = G_{\infty,\kappa}^{(d)}(\cdot\,,\cdot\,;t,1)$. Here are collected all the needed estimates:

Lemma A.1. *$\forall d \in \{1,2,3\}$, there exists a constant $C_d > 0$ s.t.*
(i). $\forall \kappa > 0$, $\forall \gamma > 0$, $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_\infty^{2d}$ and $\forall t > 0$:

$$G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,\gamma) \leq \left(\frac{\kappa}{\sinh(\kappa t)}\right)^{\frac{d}{2}} t^{\frac{d}{2}} \gamma^{\frac{d}{2}} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};\gamma t) \leq \gamma^{\frac{d}{2}} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};\gamma t) \leq (2\pi t)^{-\frac{d}{2}}, \tag{A.8}$$

$$\left|\nabla_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \sqrt{\kappa} \sqrt{\coth\left(\frac{\kappa}{2}t\right)} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,2), \tag{A.9}$$

$$\left|\Delta_{\mathbf{x}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \kappa \coth(\kappa t) G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};t,2). \tag{A.10}$$

(ii). $\forall L \in (0,\infty)$, $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$ and $\forall t > 0$:

$$\left|\nabla_{\mathbf{x}} G_{L,0}^{(d)}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \frac{(1+t)^d}{\sqrt{t}} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t), \tag{A.11}$$

$$\left|\Delta_{\mathbf{x}} G_{L,0}^{(d)}(\mathbf{x},\mathbf{y};t)\right| \leq C_d \frac{(1+t)^d}{t} G_{\infty,0}^{(d)}(\mathbf{x},\mathbf{y};2t). \tag{A.12}$$

We continue with the following lemma expressing the semigroup property in the kernels sense:

Lemma A.2. *$\forall d \in \{1,2,3\}$, $\forall \delta > 0$, $\forall t > 0$, $\forall 0 < u < t$:*
(i). $\forall \kappa \geq 0$, $\forall L \in (0,\infty]$ and $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_L^{2d}$:

$$\int_{\Lambda_L^d} \mathrm{d}\mathbf{z}\, G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{z};\delta(t-u)) G_{L,\kappa}^{(d)}(\mathbf{z},\mathbf{y};\delta u) = G_{L,\kappa}^{(d)}(\mathbf{x},\mathbf{y};\delta t). \tag{A.13}$$

(ii). $\forall \kappa > 0$, $\forall \gamma > 0$ and $\forall (\mathbf{x},\mathbf{y}) \in \Lambda_\infty^{2d}$:

$$\int_{\Lambda_\infty^d} \mathrm{d}\mathbf{z}\, G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{z};\delta(t-u),\gamma) G_{\infty,\kappa}^{(d)}(\mathbf{z},\mathbf{y};\delta u,\gamma) = \gamma^{\frac{d}{2}} G_{\infty,\kappa}^{(d)}(\mathbf{x},\mathbf{y};\delta t,\gamma). \tag{A.14}$$

Now, we give some estimates on the operator and trace norms of the semigroup $\{G_{L,\kappa}(t)\}_{t>0}$. For any $\kappa \geq 0$ and $L \in (0,\infty]$, $\{G_{L,\kappa}(t)\}_{t>0}$ is a contraction semigroup, see e.g. [20, Sec. 1.2]:

Lemma A.3. *$\forall d \in \{1,2,3\}$, $\forall \kappa \geq 0$ and $\forall t > 0$:*

$$\forall L \in (0,\infty), \quad \|G_{L,\kappa}(t)\| \leq \|G_{\infty,\kappa}(t)\| \leq (\cosh(\kappa t))^{-\frac{d}{2}} \leq 1. \tag{A.15}$$

Restricting to $\kappa > 0$, $\forall L \in (0,\infty]$ $\{G_{L,\kappa}(t)\}_{t>0}$ is a Gibbs semigroup, see [20, Sec. 3.1]:

Lemma A.4. *$\forall d \in \{1,2,3\}$, $\forall \kappa > 0$ and $\forall L \in (0,\infty]$, $\{G_{L,\kappa}(t)\}_{t>0}$ is a trace class operator on $L^2(\Lambda_L^d)$. Moreover, denoting $E_{\infty,\kappa}^{(\mathbf{0})} = d\frac{\kappa}{2}$, one has for any $L \in (0,\infty)$:*

$$\mathrm{Tr}_{L^2(\Lambda_L^d)}\{G_{L,\kappa}(t)\} \leq \mathrm{Tr}_{L^2(\Lambda_\infty^d)}\{G_{\infty,\kappa}(t)\} = \left(2\sinh\left(\frac{\kappa}{2}t\right)\right)^{-d} = \frac{\mathrm{e}^{-E_{\infty,\kappa}^{(\mathbf{0})}t}}{(1-\mathrm{e}^{-\kappa t})^d}.$$

A.2 Proof of Lemmas A.1-A.4.

Proof of Lemma A.1. From the lower bounds in (B.2)-(B.4), (A.2) is an upper bound for (A.3) what leads to (A.8). (A.9)-(A.10) are obtained by direct calculations. The crucial ingredients are:

$$\forall \mu,\nu > 0,\, \forall x \geq 0, \quad x^\mu \mathrm{e}^{-\nu x} \leq \left(\frac{2\mu}{\mathrm{e}\nu}\right)^\mu \mathrm{e}^{-\frac{\nu}{2}x}, \tag{A.16}$$

and the identity (B.6) for (A.10). (A.11)-(A.12) follow from [8, Prop. 2]. □

Proof of Lemma A.2. (i) follows from the semigroup property which reads as: $G_{L,\kappa}(t) = G_{L,\kappa}(t-u)G_{L,\kappa}(u)$ $\forall 0 \leq u \leq t$. The proof of (ii) is based on the following explicit calculation:

$$\forall a,b,c,d>0, \qquad \int_{\mathbb{R}} \mathrm{d}z\, \mathrm{e}^{-\left[a(x+z)^2+b(x-z)^2\right]}\mathrm{e}^{-\left[c(z+y)^2+d(z-y)^2\right]} = \sqrt{\pi}(a+b+c+d)^{-\frac{1}{2}}\mathrm{e}^{-\frac{b(c+d)+a(d+c)+4ab}{a+b+c+d}x^2}\mathrm{e}^{-\frac{b(c+d)+a(d+c)+4cd}{a+b+c+d}y^2}\mathrm{e}^{-2\frac{b(d-c)+a(c-d)}{a+b+c+d}xy}. \quad \text{(A.17)}$$

Then, set $a_0 := \tanh(\frac{\kappa}{2}\delta u)$, $b_0 := \coth(\frac{\kappa}{2}\delta u)$, $c_0 := \tanh(\frac{\kappa}{2}\delta(t-u))$ and $d_0 := \coth(\frac{\kappa}{2}\delta(t-u))$. From the identities in (B.7)-(B.8) and (B.5): $a_0+b_0+c_0+d_0 = 2\sinh(\kappa\delta t)\{\sinh(\kappa\delta u)\sinh(\kappa\delta(t-u))\}^{-1}$. The rest of the proof consists in using some identities involving the hyperbolic functions to simplify each one of the factor inside the exponentials in the r.h.s. of (A.17). It is (quite) easy to get:

$$\begin{gathered}(b_0(c_0+d_0)+a_0(d_0+c_0)+4a_0b_0)\,(a_0+b_0+c_0+d_0)^{-1} = 2\coth(\kappa\delta t),\\ (b_0(d_0-c_0)+a_0(c_0-d_0))\,(a_0+b_0+c_0+d_0)^{-1} = \tanh\left(\frac{\kappa}{2}\delta t\right) - \coth\left(\frac{\kappa}{2}\delta t\right). \qquad \square\end{gathered}$$

Proof of Lemma A.3. The first inequality follows from the fact that the semigroup $\{G_{L,\kappa}(t)\}_{t\geq 0}$ is increasing in L in the sense of [7, Eq. (2.39)]. The Shur-Holmgren criterion provides the estimate on the operator norms. When $\kappa > 0$, we used (A.17) (with $c = 0 = d$) along with (B.6). $\square$

Proof of Lemma A.4. Let $(\mathfrak{I}_2(L^2(\Lambda_L^d)), \|\cdot\|_{\mathfrak{I}_2})$ and $(\mathfrak{I}_1(L^2(\Lambda_L^d)), \|\cdot\|_{\mathfrak{I}_1})$, $L \in (0,\infty]$ be the Banach space of Hilbert-Schmidt and trace class operators on $L^2(\Lambda_L^d)$ respectively. We start with $d = 1$. Let $\kappa > 0$ and $t > 0$ be fixed. In view of (A.3), from (A.17) (we set $c = 0 = d$):

$$\|G_{\infty,\kappa}(t)\|_{\mathfrak{I}_2}^2 = \int_{\Lambda_\infty^1} \mathrm{d}x \int_{\Lambda_\infty^1} \mathrm{d}y \left|G_{\infty,\kappa}^{(d=1)}(x,y;t)\right|^2 = \frac{1}{2}\frac{1}{\sinh(\kappa t)} < \infty.$$

Therefore, $G_{\infty,\kappa}(t)$ is a trace class operator on $L^2(\Lambda_\infty^1)$ since $\|G_{\infty,\kappa}(t)\|_{\mathfrak{I}_1} \leq \|G_{\infty,\kappa}(\frac{t}{2})\|_{\mathfrak{I}_2}^2 < \infty$. Since $G_{\infty,\kappa}^{(d=1)}(\cdot\,,\cdot\,;t)$ is jointly continuous on Λ_∞^2, from [8, Prop. 9] it follows that:

$$\|G_{\infty,\kappa}(t)\|_{\mathfrak{I}_1} = \int_{\Lambda_\infty^1} \mathrm{d}x\, G_{\infty,\kappa}^{(d=1)}(x,x;t) = \frac{1}{2}\frac{1}{\sinh\left(\frac{\kappa}{2}t\right)}, \tag{A.18}$$

where we used the identity (B.5). By positivity of $G_{\infty,\kappa}(t)$, $\|G_{\infty,\kappa}(t)\|_{\mathfrak{I}_1} = \mathrm{Tr}_{L^2(\Lambda_\infty^1)}\{G_{\infty,\kappa}(t)\}$. The rest of the proof leans on the estimate (A.5) which leads to $\|G_{L,\kappa}(t)\|_{\mathfrak{I}_2}^2 \leq \|G_{\infty,\kappa}(t)\|_{\mathfrak{I}_2}^2$. Hence, $\forall L \in (0,\infty)$ $G_{L,\kappa}(t)$ is also a trace class operator on $L^2(\Lambda_L^1)$, and by mimicking the above arguments, its trace norm obeys $\|G_{L,\kappa}(t)\|_{\mathfrak{I}_1} = \mathrm{Tr}_{L^2(\Lambda_L^1)}\{G_{L,\kappa}(t)\} \leq \|G_{\infty,\kappa}(t)\|_{\mathfrak{I}_1}$. The case of $d = 1$ is done. The generalization to $d = 2, 3$ is straightforward due to (A.4). $\square$

B Some useful identities and inequalities.

Here, we collect some miscellaneous inequalities/identities involving the hyperbolic functions. Most of them can be found in [1, Sec. 4.5]. For any real $\alpha \geq 0$:

$$1 \leq \cosh(\alpha) \leq \mathrm{e}^{\alpha}, \tag{B.1}$$

$$\alpha \leq \sinh(\alpha) \leq \frac{1}{2}\mathrm{e}^{\alpha}, \tag{B.2}$$

$$0 \leq \tanh(\alpha) \leq 1, \tag{B.3}$$

$$\frac{1}{\alpha} \leq \coth(\alpha) := \frac{1}{\tanh(\alpha)} \leq \frac{1+\alpha}{\alpha}, \quad \alpha > 0. \tag{B.4}$$

For any reals $\alpha > 0$ and $t > s > 0$:

$$\sinh(\alpha t) = 2\sinh\left(\frac{\alpha}{2}t\right)\cosh\left(\frac{\alpha}{2}t\right), \tag{B.5}$$

$$\coth(\alpha t) = \frac{1}{2}\coth\left(\frac{\alpha}{2}t\right) + \frac{1}{2}\tanh\left(\frac{\alpha}{2}t\right), \tag{B.6}$$

$$\coth(\alpha s) + \coth(\alpha(t-s)) = \frac{\sinh(\alpha t)}{\sinh(\alpha s)\sinh(\alpha(t-s))}, \tag{B.7}$$

$$\tanh(\alpha s) + \tanh(\alpha(t-s)) = \frac{\sinh(\alpha t)}{\cosh(\alpha s)\cosh(\alpha(t-s))}, \tag{B.8}$$

$$\tanh(\alpha s) + \tanh(\alpha(t-s)) = \tanh(\alpha t)\left\{1 + \tanh(\alpha s)\tanh(\alpha(t-s))\right\} \geq \tanh(\alpha t). \tag{B.9}$$

References

[1] Abramowitz M., Stegun I., *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, 9th Priniting with corrections, Dover Publications, Inc., New York, 1970

[2] Angelescu N., Bundaru M., Nenciu G., *On the perturbation of Gibbs semigroups*, Commun. Math. Phys. **42**, 29–30 (1975)

[3] Beau M., Savoie B., *The ideal Bose gas in open harmonic trap systems and its condensation revisited*, preprint arXiv:1306.3639

[4] Berezin F.A., Shubin M.A., *The Schrödinger Equation*, Kluwer Academic Publishers, Dordrecht, 1991

[5] Briet P., Cornean H.D., Louis D., *Diamagnetic expansions for perfect quantum gases*, J. Math. Phys. **47**(8), 083511 (2006)

[6] Briet P., Cornean H.D., Louis D., *Diamagnetic expansions for perfect quantum gases II: Uniform bounds*, Asymptotic Analysis **59**(1-2), 109–123 (2008)

[7] Broderix K., Hundertmark D., Leschke H., *Continuity properties of Schrödinger semigroups with magnetic fields*, Rev. Math. Phys. **12**, 181–225 (2000)

[8] Cornean H.D., *On the magnetization of a charged Bose gas in the canonical ensemble*, Commun. Math. Phys. **212**(1), 1–27 (2000)

[9] Cornean H.D., Nenciu G., *The Faraday effect revisited: Thermodynamic limit*, J. Funct. Anal. **257**(7), 2024–2066 (2009)

[10] Cornean H.D., Fournais S., Frank R., Hellfer B., *Sharp trace asymptotics for a class of 2D-magnetic operators*, preprint arXiv:1108.0777

[11] Hille E., Phillips R.S., *Functional Analysis and Semi-Groups*, Revised and Expanded Edition, AMS Colloquium Publications Vol. 31, American Mathematical Society, Providenc, Rhode Island, 1957

[12] Kubo R., *Statistical Mechanics, An advance Course with Problems and Solutions*, First Edition, North-Holland Physics Publishing, Amsterdam, 1965

[13] Pitaevskii L.P., Stringari S., *Bose-Einstein Condensation*, Oxford University Press, 2003

[14] Reed M., Simon B., *Methods of Modern Mathematical Physics, II : Fourier Analysis, Self-Adjointness*, Academic Press, Inc., San Diego, 1975

[15] Reed M., Simon B., *Methods of Modern Mathematical Physics, IV : Analysis of Operators*, Academic Press, Inc., San Diego, 1978

[16] Ruelle D., *Statistical Mechanics, Rigorous results*, W.A. Benjamin, Inc., New York, Amsterdam, 1969

[17] Savoie B., *On the atomic orbital magnetism: A rigorous derivation of the Larmor and Van Vleck contributions*, preprint arXiv:1302.1054

[18] Simon B., *Schrödinger semigroups*, Bull. Amer. Math. Soc. (N.S.) **7**(3), 447–526 (1982). Erratum:*ibid.* **11**(2), 426–426 (1984)

[19] Uhlenbrock D., *Perturbation of statistical semigroups in quantum statistical mechanics*, J. Math. Phys. **12**, 2503–2512 (1971)

[20] Zagrebnov V.A., *Topics in the Theory of Gibbs Semigroups*, Leuven Notes in Mathematical and Theoretical Physics, Vol. 10–Serie A, Leuven Academic Press, Leuven, 2003